University of Tikrit

Chemical Engineering Department

Basic Principles and Calculations in Chemical Engineering

First Year

By

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Part 2

Material Balances

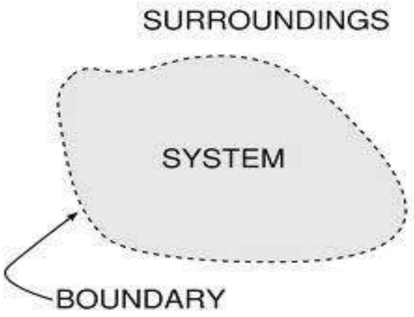
Chapter 6

Introduction to Material Balance:

Material balance involves calculations the quantities of all materials that enter and leave any system or process which are based on the principle of the **"law of conversation of mass**". This law states that matter is neither created nor destroyed in the process and the total mass remains unchanged. The general principle of material balance calculations is to put and solve a number of independent equations involve number of unknowns of compositions and mass flow rates of streams enter and leave the system or process.

The **process** can be defined as one or a series of operations in which physical and chemical treatments are carried out and a desired product is result in the end such as distillation, drying, absorption, chemical manufacture, … etc.

The **system** can be defined as any arbitrary portion of a process that you want to consider for analysis such as a reactor. The **system boundary** must be fixed in each problem by drawing an imaginary boundary around it as shown in the following figure:



There are two important classes of systems:

1. **Closed system:**
   The material neither enters nor leaves the vessel (system), as shown below:

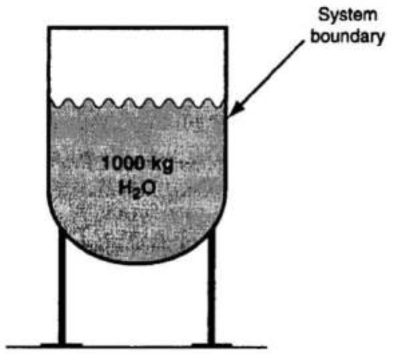


Figure 1: Closed system

2. **Open system (flow system):**
   The material cross the system boundary, as shown below:

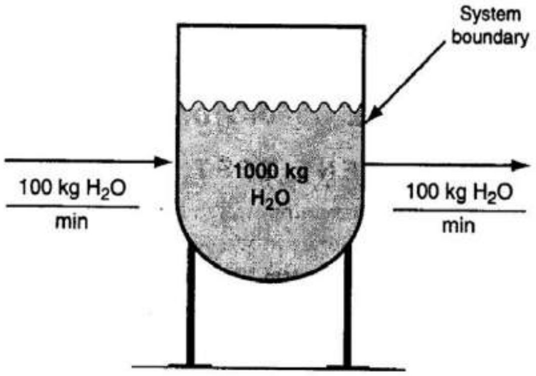


Figure 1: Open system (Flow system)

The chemical processes can be classified as **batch, continuous and semi-batch**:

1. **Batch process:**

The feed materials are placed into the system (reactor, mixer, filter,….etc) at the beginning of the process. These materials are held for a period of time known as "**residence time**" or " **retention period**" during which the required physical and/or chemical changes are occurred. The products are removed all at once after this time. No masses crossed the system boundary during this time. Batch process fall into the category of closed systems.

The basis used in such processes is usually "**one batch**", and the material balance for physical batch processes in which there is no chemical reaction can be written as:

Input	**=**	**Output**
(Initial quantity)		**(Final quantity)**

This equation can be applied for every substance (component balance) or for total materials (total material balance).

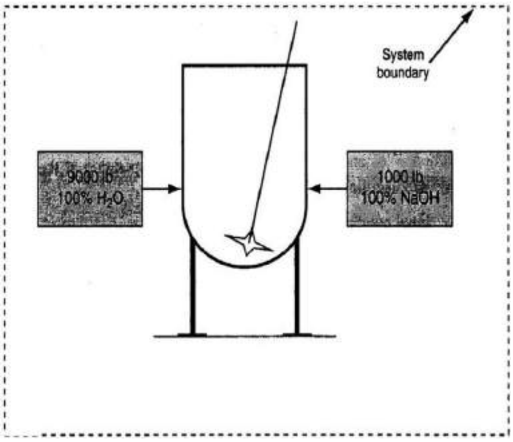


Figure 2: The **initial** state of a batch mixing process

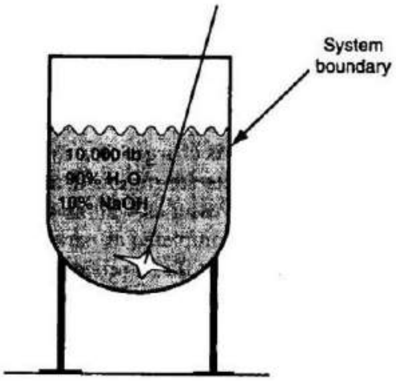


Figure 3: The **final** state of a batch mixing process

2. Semi-batch process:

A semi-batch reactor of stirred type tank as shown in the **Figure 4**, often used for its own particular characteristics. In this type, all quantity of one reactant is initially put in the reactor, and then other reactants are continuously fed. Only flows enter the systems, and no leave, hence the system is an unsteady state. This arrangement is useful when the heat of reaction is large. The heat evolved can be controlled by regulating the rate of addition of one of the reactants.

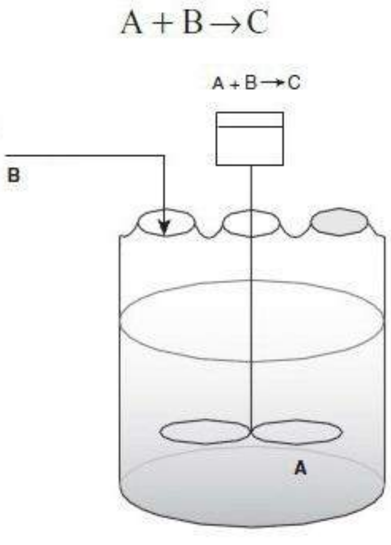


Figure 4: Semi-batch reactor (Stirred type reactor)

3. Continuous process (Flow process):

The input and output materials are continuously transferred across the system boundary; i.e. the feed continuously enters the system and the product continuously leaves the system. The physical and/or chemical changes take place during the flow of materials through the effective parts of equipments (packing, sieve plate, filter cloth,…etc). A convenient period of time such as minute, hour, or day must chosen as a basis over which material balance calculations be made.

This type of processes can be classified as "**steady state**" and "**unsteady state**" processes.

a- Steady state process:

The steady state process can be defined as that process in which all the operating conditions (temperature, pressures, compositions, flow rate,…..etc.) remains constant with time. In such process there is no accumulation in the system, and the equation of material balance can be written as:

$$\boxed{\textbf{Input} = \textbf{Output}}$$

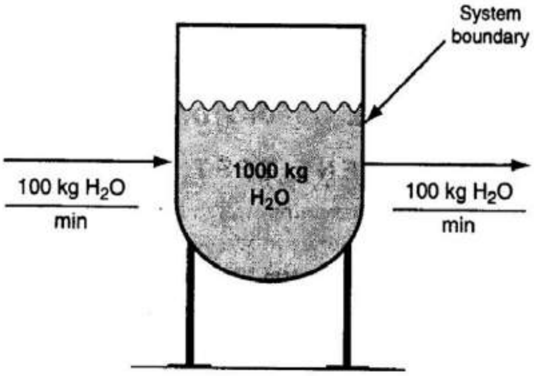


Figure 5: Steady state system

b- Unsteady state process:

For an unsteady state process, not all of the operating conditions in the process (e.g., temperature, pressure, compositions, flow rate,… etc.) remain constant with time, and/or the flows in and out of the system can vary with time, hence the accumulation of materials within can be written as follows:

$$\boxed{\textbf{Input} - \textbf{Output} = \textbf{Accumulation}}$$

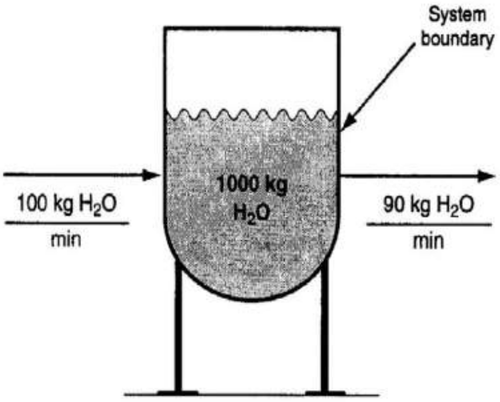


Figure 6: Initial conditions for an open unsteady state system with accumulation.

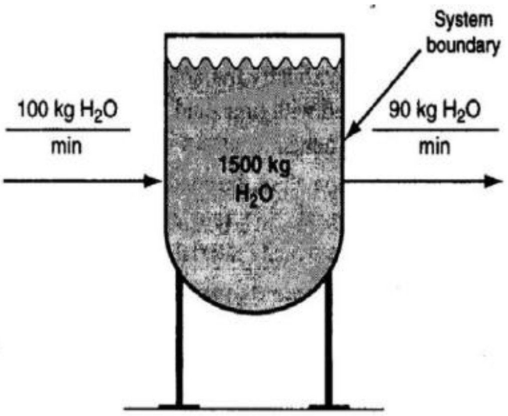


Figure 7: The condition for the open unsteady state system with accumulation after 50 min.

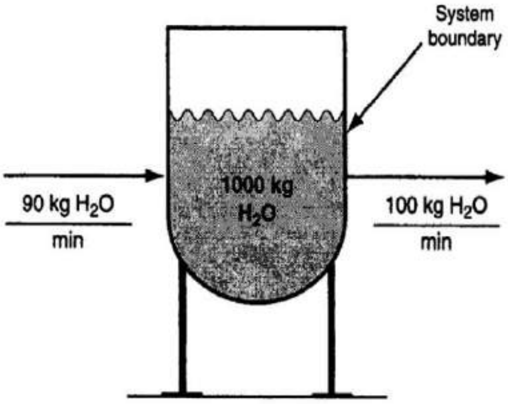


Figure 8: Initial conditions for an unsteady state process with negative accumulation.

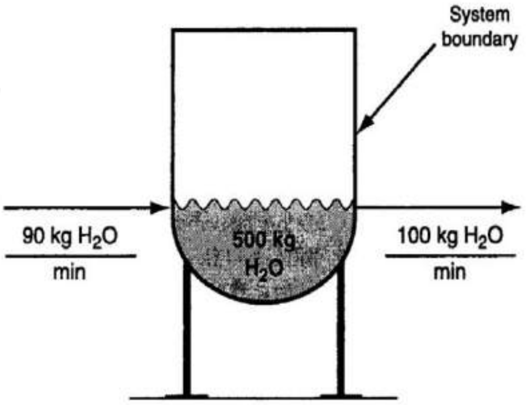


Figure 9: Condition of the open unsteady state system with negative accumulation after 50 min.

Remarks:

1. By their nature, batch and semi-batch processes are unsteady state operations since the concentration within the closed system is continuously changed with time.
2. Continuous processes are usually runs as close as possible to the steady state by using suitable control units. However, unsteady state (transient) conditions exist during the start up of a process. All material balance and design calculations are done for steady state conditions.
3. Batch processes are commonly used for small scale processes in which relatively small quantities of a product are to be produced, while continuous process is better suited to large production rates.
4. All material balance calculations in this chapter are made on steady state processes in which the **accumulation term is zero**. However, material balance on a batch process can be made over a residence time and on the basis of one batch (integral balance).

5. Calculations of unsteady state processes are somewhat more complicated than that of the steady state processes since involving differential equations which can be solve by integration. These calculations with their applications in many chemical engineering fields (mass transfer, heat transfer, chemical kinetics,…etc.) will be given in "Applied Mathematics in Chemical Engineering" within 3rd year of study.

Chapter 7

A general Strategy for Solving Material Balance Problems

The strategy outlined below is designed to focus your attention on the main path rather than the detours:

1. **Read and understand the problem statement**
   This mean read the problem carefully so that you know what is given and what is to be accomplished.
2. **Draw a sketch of the process and specify the system boundary**
   Draw a simplified imaginary sketch (block diagram) or a flow sheet or process flow diagram (PFD) consists of boxes which represent equipments, and lines which indicate all streams enter and leaves each equipment.
3. **Label the flow of each stream and the associated compositions with symbols**
   Put a letter as a symbol stream such as (**F**) for feed stream, (**P**) for product stream….etc. Furthermore, put all the known values of compositions and stream flows on the figure by each stream; calculate additional compositions from the given data as necessary.

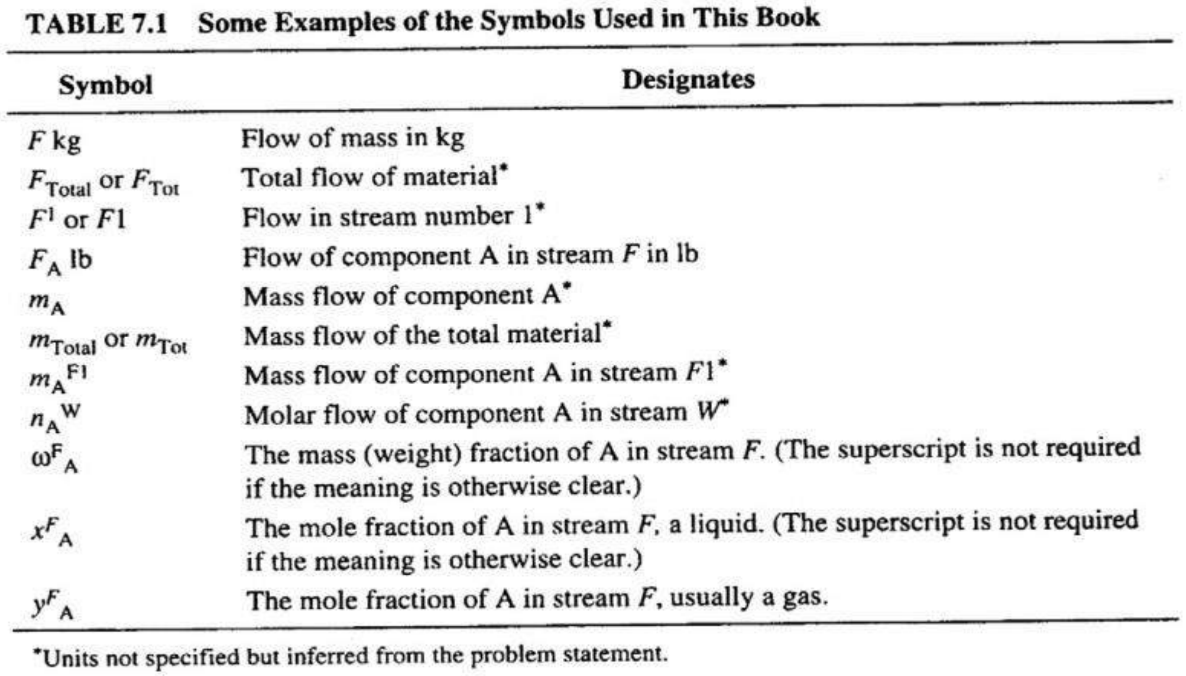


TABLE 7.1 Some Examples of the Symbols Used in This Book

Symbol	Designates
F kg	Flow of mass in kg
F_{Total} or F_{Tot}	Total flow of material*
F^1 or $F1$	Flow in stream number 1*
F_A lb	Flow of component A in stream F in lb
m_A	Mass flow of component A*
m_{Total} or m_{Tot}	Mass flow of the total material*
m_A^{F1}	Mass flow of component A in stream $F1$*
n_A^W	Molar flow of component A in stream W*
$\omega^F{}_A$	The mass (weight) fraction of A in stream F. (The superscript is not required if the meaning is otherwise clear.)
$x^F{}_A$	The mole fraction of A in stream F, a liquid. (The superscript is not required if the meaning is otherwise clear.)
$y^F{}_A$	The mole fraction of A in stream F, usually a gas.

*Units not specified but inferred from the problem statement.

Example 7.2: A continuous mixer mixes NaOH with H_2O to produce an aqueous solution of NaOH. Determine the composition and flow rate of the product if the flow rate of NaOH is 1000 kg/hr, and the ratio of the flow rate of the H_2O to the product solution is 0.9.

We will use this example in subsequent illustrations of the proposed strategy. For this example, just a sketch of the process is required.

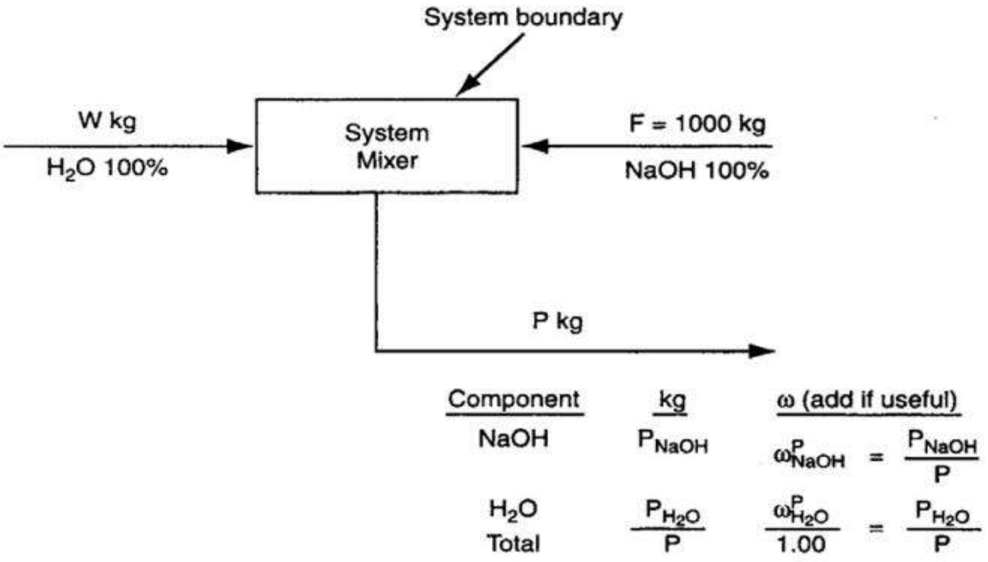


Figure E7.3

4. **Write additional data** required to solve the problem and the chemical equations if the process involves chemical reaction.
5. **Select a suitable basis of calculations**.
6. **List by symbols each of the unknown values** of the stream flows and compositions
7. **Make a number of independent material balances equations** equal to unknown quantities to be calculated. It is important to put these equations in proper sequence so that the first one content only one unknown in order to avoid complicated solution of the simultaneous equations. Three type of material balance equations can be formulated:

   a. Equation for total quantities which is called (**total material balance**) or (**over all material balance**).
   b. Equation for each component which is called (**component material balance**). If there is no chemical reaction the number of equations that can be written is equal to the number of components in the system.
   c. Equation for each element which is called (**element material balance**) if there is a chemical reaction.

8. The existence of a substance that enters in one inlet stream and leaves in one outlet stream with known compositions and it passes unchanged through the process unit (inert for chemical reaction) is greatly simplified material balance calculations. This substance is termed as (**tie component**). It is important to search for the existence of a tie component and formulate a material balance equation. Nitrogen is considered as a tie component in handling of combustion calculations. Since it is input within air stream,

unreacted, and out with the exit flue gases. If there are more than on tie component in the same input and output streams, these components can be made on (**over all tie components material balance**).

9. Check your answers by introducing them, or some of them, into the material balance equations. Are the equations satisfied? Are the answers reasonable?

Chapter 8

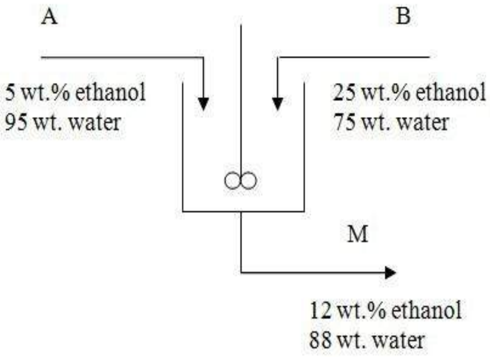
Solving Material Balance Problems for Single Units Without Reaction

1. Mixer unit:

Example: It is required to prepare 1250 kg of a solution composed of 12 wt.% ethanol and 88 wt.% water. Two solutions are available, the first contains 5 wt.% ethanol, and the second contains 25 wt.% ethanol. How much of each solution are mixed to prepare the desired solution?

Solution:

1. **Ethanol balance**



Input = output

$$\mathrm{A}\left(\frac{5}{100}\right) + \mathrm{B}\left(\frac{25}{100}\right) = \mathrm{M}\left(\frac{12}{100}\right)$$

$$0.05\ \mathrm{A} + 0.25\ \mathrm{B} = 0.12\ \mathrm{M}$$

$$\mathrm{A} = \left(\frac{150 - 0.25\ \mathrm{B}}{0.05}\right) = 3000 - 5\,B \ldots\ldots\ldots..(\mathbf{1})$$

2. **Water balance**

Input = output

$$0.95\ \mathrm{A} + 0.75\ \mathrm{B} = 0.88\ \mathrm{M} = 0.88\ (1250) = 1100$$

$$0.95\ \mathrm{A} + 0.75\ \mathrm{B} = 1100 \ldots\ldots\ldots..(\mathbf{2})$$

Sub. (1) in (2)

0.95(300-5 B) + 0.75 B = 1100

2850 - 4.75 + 0.75 B =1100

4 B =1750 …………………. B= 437.5 kg

Sub. B in (1) : A= 3000 – 5(437.5) = 812.5 kg

3. **Checking:** Total material balance (T.M.B.), Input = A + B = 437.5 + 812.5 =1250 kg
Output = M= 1250 kg

2. **Extraction unit**:

Example 8.1: Extraction of Streptomycin from a Fermentation Broth**:**

Streptomycin is recovered by contacting the fermentation broth with an organic solvent in an extraction process. The extraction process is able to recover the Streptomycin because Streptomycin has a greater affinity for dissolving in the organic solution than in the aqueous solution. Figure E8.1 shows the overall process. Determine the mass fraction of Streptomycin in the exit organic solvent assuming that no water exits with the solvent and no solvent exits with the aqueous solution. Assume that the density of the aqueous solution is 1 g/cm^3 and the density of the organic solvent is 0.6 g/cm^3.

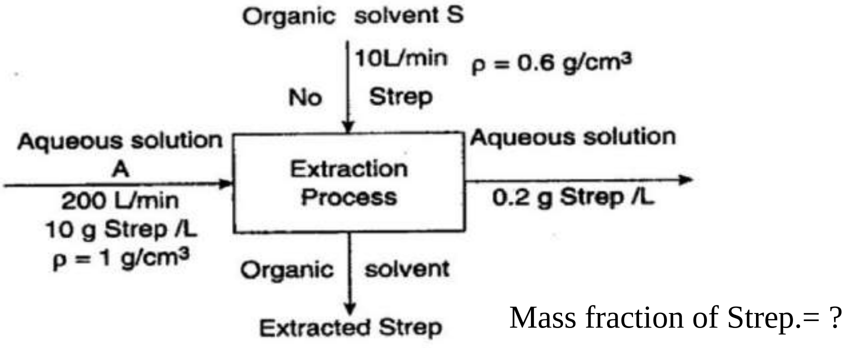


Figure E8.1

Solution:

This is an open (flow), steady-state process without reaction. Assume because of the low concentration of Strep. In the aqueous and organic fluids that the flow rates of the entering fluids equal the flow rates of the exit fluids.

Basis: 1 min

The material balances are *in* = *out* in grams. Let x be the g of Strep per L of solvent S.

Strep. balance:

$$\frac{200 \text{ L of A}}{}\left|\frac{10 \text{ g Strep}}{1 \text{ L of A}}\right. + \frac{10 \text{ L of S}}{}\left|\frac{0 \text{ g Strep}}{1 \text{ L of S}}\right. = \frac{200 \text{ L of A}}{}\left|\frac{0.2 \text{ g Strep}}{1 \text{ L of A}}\right. + \frac{10 \text{ L of S}}{}\left|\frac{x \text{ g Strep}}{1 \text{ L of S}}\right.$$

$$x = 196 \text{ g Strep/L of S}$$

To get the g Strep/g solvent, use the density of the solvent:

$$\frac{196 \text{ g Strep}}{1 \text{ L of S}}\left|\frac{1 \text{ L of S}}{1000 \text{ cm}^3 \text{ of S}}\right|\frac{1 \text{ cm}^3 \text{ of S}}{0.6 \text{ g of S}} = 0.3267 \text{ g Strep/g of S}$$

$$\text{The mass fraction Strep} = \frac{0.3267}{1 + 0.3267} = 0.246$$

3. **Membrane unit**:

Example 8.2: Separation of Gases Using a Membrane**:**

Membranes represent a relatively new technology for the separation of gases. One use that has attracted attention is the separation of nitrogen and oxygen from air. Figure E8.2a illustrates a nanoporous membrane that is made by coating a very thin layer of polymer on a porous graphite supporting layer. What is the composition of the waste stream if the waste stream amounts to 80% of the input stream?

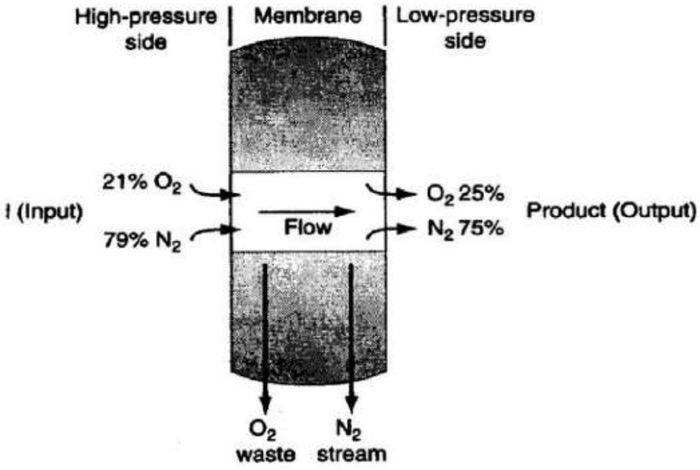


Figure E8.2a

Solution:

This is an open, steady-state process without chemical reaction. The system is the membrane as depicted in Figure E8.2. Let y_{O_2} be the mole fraction of oxygen as depicted in Figure E8.2, y_{N_2} be the mole fraction of nitrogen, and let n_{O_2} and n_{N_2} be the respective moles.

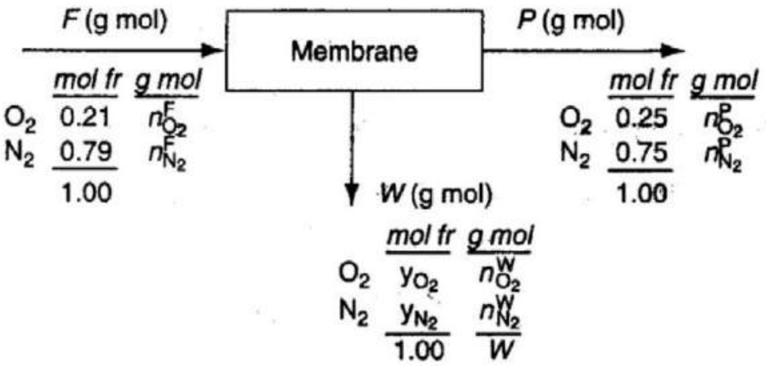


Figure E8.2b

Basis: F=100 gmole
Input = Output
F = P + W
W = 80% F = 0.8 x 100 = 80 gmole
P= 20 gmole

Specifications: $n^F_{O_2} = 0.21(100) = 21$ gmole

$n^F_{N_2} = 0.79(100) = 79$ gmole

$y^P_{O_2} = n^P_{O_2}/P = 0.25 \qquad n^P_{O_2} = 0.25P = 5$ gmole

$y^P_{N_2} = n^P_{N_2}/P = 0.75 \qquad n^P_{N_2} = 0.75P = 15$ gmole

Oxygen Material Balance (O_2 M.B):

$$0.21\,(100) = 0.25P + y^W_{O_2}\,(80)$$

$$0.21\,(100) = 0.25(20) + n^W_{O_2} \Longrightarrow n^W_{O_2} = 16 \text{ gmole}$$

Nitrogen Material Balance (N_2 M.B):

$$0.79\,(100) = 0.75P + y^W_{N_2}\,(80)$$

$$0.79\,(100) = 0.75(20) + n^W_{N_2} \Longrightarrow n^W_{N_2} = 64 \text{ gmole}$$

Mole fraction of O_2 in waste, $y^W_{O_2} = \frac{16}{16+64} = 0.2$

Mole fraction of N_2 in waste, $y^W_{N_2} = \frac{64}{16+64} = 0.8$

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4. **Distillation column**:

Example : Overall Analysis for a Continuous Distillation Column**:**

A binary mixture consists of 35 % benzene and 65 % toluene are continuously fed to the distillation column at a rate of 1000 kg/hr. Whereas, the distillate flow rate was 10% from the feed flow rate. The distillate (top product) contains 85 % benzene. Calculate quantity and compositions of the waste stream.

Solution:

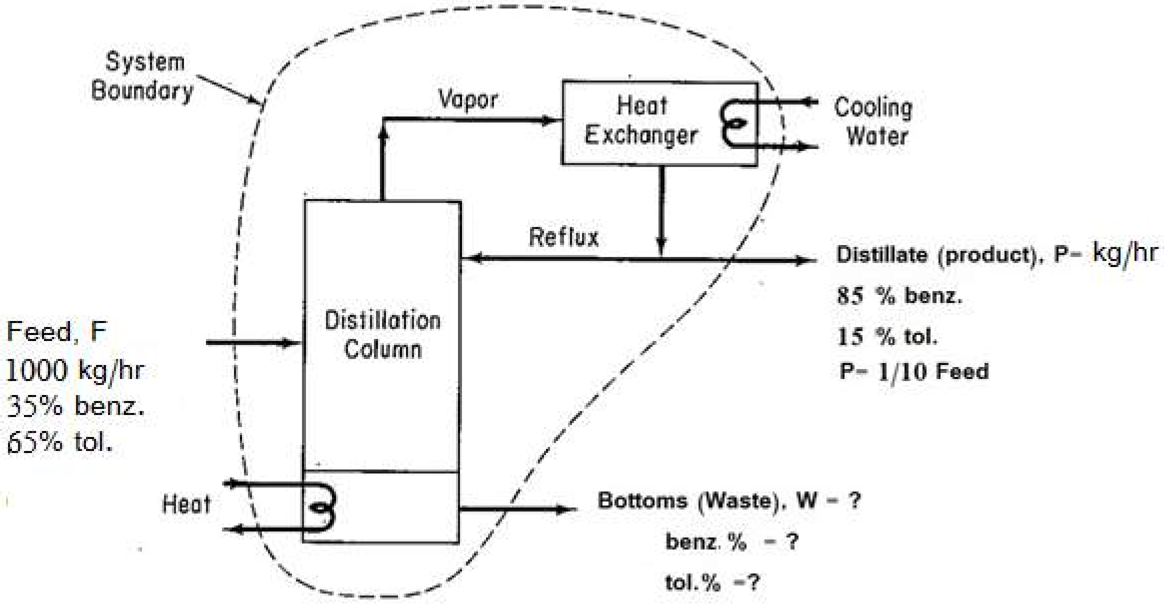
Although the distillation unit shown in Figure below is comprised of more than one unit of equipment, you can select a system that includes all of the equipment inside the system boundary. Consequently, you can ignore all the internal streams for this problem.

Basis: 1 hr
F = 1000 kg
P = (10 /100) of Feed = 0.1 x (1000) = 100 kg

Overall Material Balance:

Input = Output

$F = P + W \Longrightarrow 1000 = 100 + W \Longrightarrow W = 900$ kg



Benzene Material Balance:

(0.35) (1000) = (0.85) (100) + Kg of benz. in (W)

350 = 85 + Kg of benz. in (W) ⟹ Kg of benz. in (W) = 265 kg

Toluene Material Balance:

(0.65) (1000) = (0.15) (100) + Kg of tol. in (W)

650 = 15 + Kg of benz. in (W) ⟹ Kg of tol. in (W) = 635 kg

W = Kg of benz. in (W) + Kg of tol. in (W) = 265 + 635 = 900 kg

Mass fraction of benz. in waste = $\frac{265}{265+635} = 0.294$

Mass fraction of tol. in waste = $\frac{635}{265+635} = 0.706$

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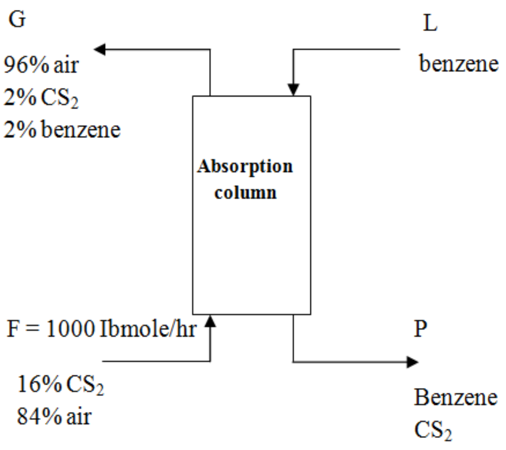
5. Absorption column:

Example : A gaseous mixture (F) consists of 16 mol% CS_2 and 84 mol% air are fed to the absorption column at a rate of 1000 Ibmole/hr. Most of the CS_2 input are absorbed by liquid benzene (L) which is fed to the top of the column. 1 % of benzene input are evaporated and out with the exit gas stream which consists of 96 mol% air, 2 mol% CS_2 and 2 mol% benzene. The product liquid stream (P) consists of benzene and CS_2. Calculate the mole flow rates of (G), (L) and (P) and the compositions.

Solution:



Basis = 1 hr
F = 1000 Ibmole

<u>Air material balance</u>: (Tie component)
(0.84) (F) = (0.96) (G)
(0.84)(1000) = (0.96) (G)
G = 840/0.96 = 875 Ibmole

<u>Benzene material balance</u>:
Benzene in (G) = (875) (0.02) = 17.5 Ibmole
17.5 = 1% of benzene input
17.5 = (0.01) (L) $\Longrightarrow$ L = 1750 Ibmole

Benzene in (P) = 99% of benzene input = (0.99) (L) =(0.99) (1750) = 1732.5 Ibmole

Let x = mole fraction of benzene in (P) $\Longrightarrow$ P x = 1732.5 ……………...(1)

<u>CS_2 material balance</u>:
(0.16) (F) = (0.02) (G) + P (1-x)
(0.16) (1000) = (0.02) (875) + P – P x
160 =17.5 + P – 1732.5 $\Longrightarrow$ P = 1875 Ibmole

Sub. (P) in equation (1):
x = (1732.5) / (1875) = 0.924 mole fraction of benzene in (P)
mole fraction of CS_2 in (P) = 1- 0.924 = 0.076

<u>Checking total material balance:</u>
Input = F + L = 1000 + 1750 = 2750 Ibmole
Output = G + P = 875 + 1875 = 2750 Ibmole

Example 8.4 : Mixing of battery (Sulfuric) Acid **:**

You are asked to prepare a batch of 18.63% battery acid as follows. A tank of old weak battery acid (H_2SO_4) solution contains 12.43% H_2SO_4 (the remainder is pure water). If 200 kg of 77.7% H_2SO_4 is added to the tank, and the final solution is to be 18.63% H_2SO_4, how many kilograms of battery acid have been made? See Figure E8.4.

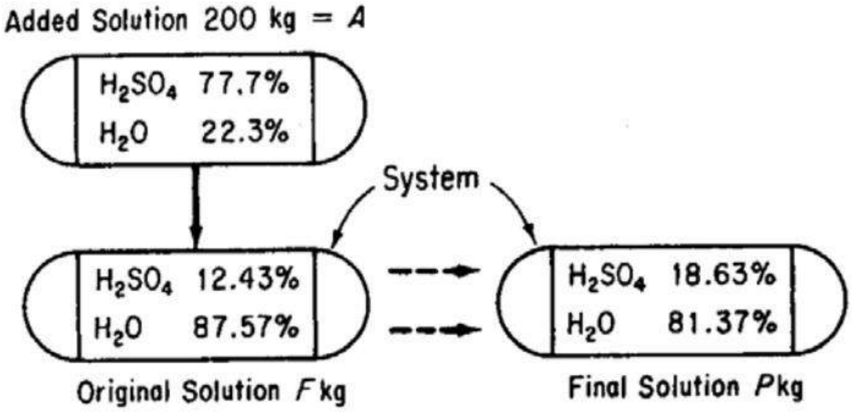


Figure E8.4

Solution:

Overall material balance:

Input = Output

A + F = P
200 + F = P ………………(1)

H_2SO_4 material balance:

(0.777) (200) + (0.1243) (F) = (0.1863) (P) ……………..(2)

H_2O material balance:

(0.223) (200) + (0.8757) (F) = (0.8137) (P)………………(3)

From equation(1), P = 200 + F

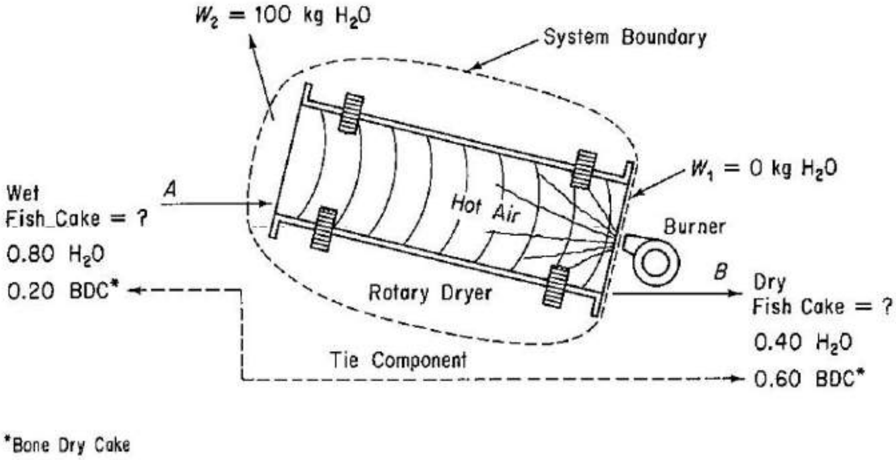
Sub. Equation (1) in (2):

(0.777) (200) + (0.1243) (F) = (0.1863) (200 + F)
155.4 + 0.1243 **F** – 37.26 = 0.1863 **F**
F= 1905.5 kg & **P** =2105.5 kg

Example 8.5 : Dryer **:**

In the processing of the fish, after the oil is extracted, the fish cake is dried in rotary drum dryers, finely ground, and packed. The resulting product contains 65% protein. In a given batch of fish cake that contains 80% water (the remainder is dry cake), 100 kg of water is removed, and it is found that the fish cake is then 40% water. Calculate the weight of the fish cake originally put into the dryer.

Solution:



Basis: 100 kg water evaporated

Overall material balance:

Input = Output

$A + W_1 = B + W_2$

$A + 0 = B + 100 \Longrightarrow A = B + 100$ …………….. (1)

BDC material balance:

Input = Output

$(0.2)(A) = (0.6)(B) \Longrightarrow B = (1/3)A$ …………….(2)

Sub. Eq. (2) into (1):

$A = (1/3)A + 100 \Longrightarrow A = 150$ kg initial cake

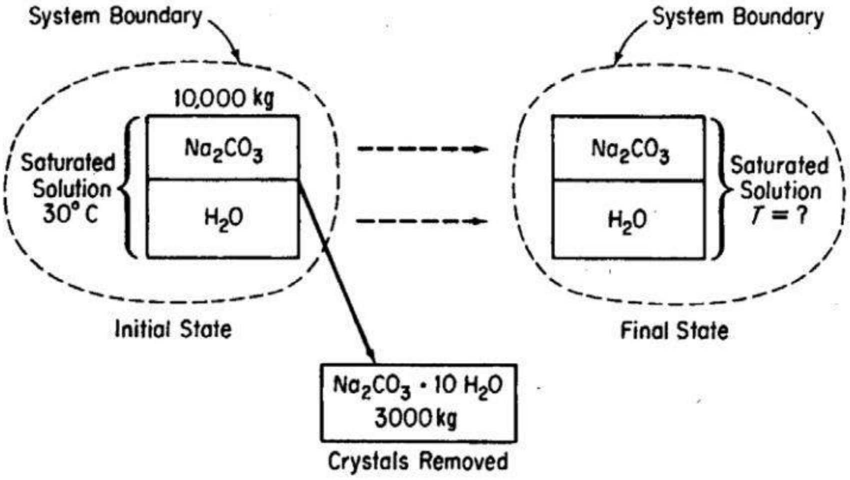
$B = (1/3)A = (1/3)(150) = 50$ kg

Example 8.6 : Crystallization **:**

A tank holds 10,000 kg of a saturated solution of Na_2CO_3 at 30°C. You want to crystallize from this solution 3000 kg of $Na_2CO_3.10H_20$ without any accompanying water. To what temperature must the solution be cooled? The solubility data of Na_2CO_3 as a function of the temperature is given as below:

Temp. (^oC)	Solubility (g Na_2CO_3 / 100 g H_2O)
0	7
10	12.5
20	21.5
30	38.8

Solution:



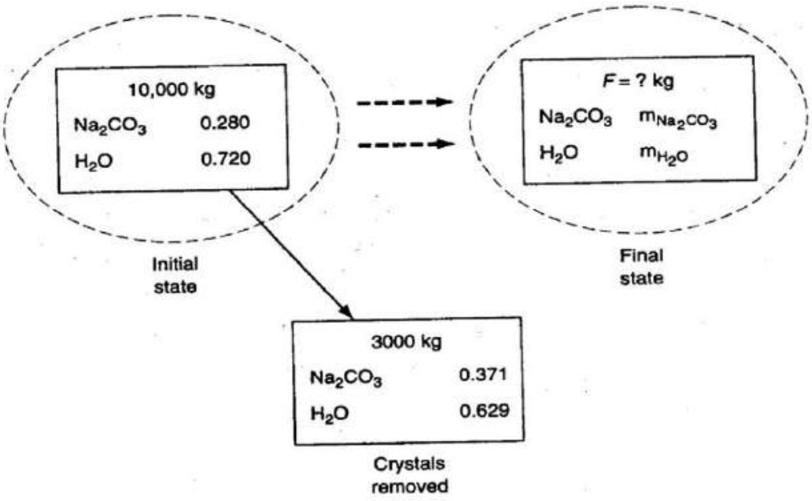
Since the initial solution is saturated at 30^{o}C, you can calculate the composition of the initial solution:

$$\text{Mass fraction of } \mathrm{Na_2CO_3} = \frac{38.8 \text{ g } \mathrm{Na_2CO_3}}{38.8 \text{ g } \mathrm{Na_2CO_3} + 100 \text{ g } \mathrm{H_2O}}$$

Basis: 1 g mol of $Na_2CO_3.10H_20$

Comp.	Mol	Mol wt.	Mass	Mass fraction
Na_2CO_3	1	106	106	0.371
H_20	10	18	180	0.629
Total			286	1.0

Basis: 10000 kg of saturated solution at 30^{o}C



Because we are treated this problem as an unsteady-state problem (the flow = 0), the mass balance reduces to:

Overall material balance:

Initial state – Final state = Crystal removed

10000 – F = 3000 ⟹ F = 7000 kg

Na_2CO_3 material balance:
(0.28) (10000) - ($\mathbf{M}_{\_Na_2CO_3}$) (F) = (0.371) (3000) , where: **M**=mass fraction

(0.28) (10000) - ($\mathbf{M}_{\_Na_2CO_3}$) (7000) = (0.371) (3000)

$\mathbf{M}_{\_Na_2CO_3}$ = 0.241

Mass of Na_2CO_3 in the final state = ($\mathbf{M}_{\_Na_2CO_3}$) (F) = (0.241) (7000) = **1687 kg**

H_2O material balance:
(1-0.28) (10000) - ($\mathbf{M}_{\_H_2O}$) (F) = (0.629) (3000)

(0.72) (10000) - ($\mathbf{M}_{\_H_2O}$) (7000) = (0.629) (3000)

$\mathbf{M}_{\_H_2O}$ = 0.759

Mass of H_2O in the final state = ($\mathbf{M}_{\_H_2O}$) (F) = (0.759) (7000) = **5313 kg**

To find the temperature of the final solution, calculate the composition of the final solution in terms of (g Na_2CO_3. / 100 g H_2O) so that you can use the tabulated solubility data listed above.

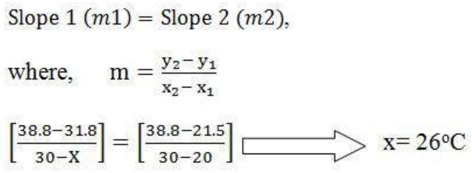
$$\frac{1687 \text{ kg } Na_2CO_3}{5313 \text{ kg } H_2O} = \frac{31.8 \text{ g } Na_2CO_3}{100 \text{ g } H_2O}$$

Na_2CO_3	H_2O
1687 kg	5313 kg
X	100 g

⟹ X =31.8

Thus, the temperature to which the solution must be cooled lies between 20^{o}C and 30^{o}C. By linear interpolation:

$$(30^o\,\mathrm{C}) - \left[\frac{38.8 - 31.8}{38.8 - 21.5}\right](10^o\,\mathrm{C}) = 26^o\,\mathrm{C}$$



Slope 1 ($m1$) = Slope 2 ($m2$),

where, $m = \frac{y_2 - y_1}{x_2 - x_1}$

$$\left[\frac{38.8-31.8}{30-X}\right] = \left[\frac{38.8-21.5}{30-20}\right] \Longrightarrow x = 26^o\mathrm{C}$$

Home work:

Problems: 8.1, 8.5, 8.8, 8.11, 8.12, 8.13, 8,18, 8.22.

Chapter 9

The Chemical Reaction Equation and Stoichiometry

Stoichiometry:

When chemical reactions occur, in contrast with physical changes of material such as evaporation or dissolution, you want to be able to predict the mass or moles required for the reaction(s), and the mass or moles of each species remaining after the reaction has occurred. Reaction stoichiometry allows you to accomplish this task. The word stoichiometry (stoi-ki-om-e-tri) derives from two Greek words: stoicheion (meaning "element") and metron (meaning "measure"). **Stoichiometry provides a quantitative means of relating the amount of products produced by chemical reactions to the amount of reactants**.

The following expressions are widely used in stoichiometry:

1. **Stoichiometric coefficients:**
   The numbers that are precede the chemical substances involved in the chemical reaction equation are known as " stoichiometric coefficients". These coefficients represent quantity of any reactant that is theoretically required for complete conversion of other reactants.

2. **Stoichiometric ratios:**
   The ratio between any stoichiometric coefficients in a balanced chemical equation is known as " stoichiometric ratio".

   As an example the reaction of nitrogen and hydrogen to produce ammonia:
   $N_2 + 3H_2 \rightarrow 2NH_3$
   The stoichiometric ratios of $N_2/H_2 = 1/3$, $N_2/NH_3 = 1/2$ and $H_2/NH_3 = 3/2$

Example 9.2: Use of the Chemical Equation to Calculate the Mass of Reactants Given the Mass of Products

In the combustion of heptane, CO_2 is produced. Assume that you want to produce 500 kg of dry ice per hour, and that 50% of the CO_2 can be converted into dry ice, as shown in Figure E9.2. How many kilograms of heptane must be burned per hour?

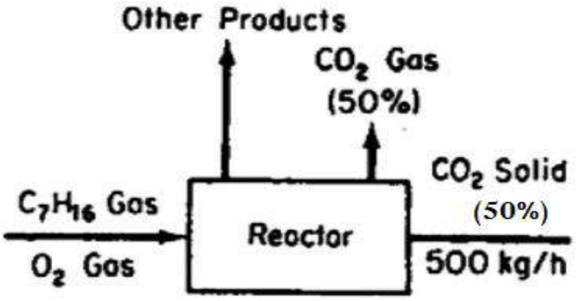


Figure E9.2

Solution:

The chemical equation is:

$C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$

Basis: 500 kg dry ice (equivalent to 1 hr)

M.wt. of CO_2 = 44 kg/kgmol & C_7H_{16} = 100.1 kg/kgmol

$$\frac{500\text{ kg dry ice}}{} \left| \frac{1\text{ kg }CO_2}{0.5\text{ kg dry ice}} \right| \frac{1\text{ kg mol }CO_2}{44.0\text{ kg }CO_2} \left| \frac{1\text{ kg mol }C_7H_{16}}{7\text{ kg mol }CO_2} \right.$$

$$\left| \frac{100.1\text{ kg }C_7H_{16}}{1\text{ kg mol }C_7H_{16}} \right. = 325\text{ kg }C_7H_{16}$$

<u>Example 9.3:</u> Application of Stoichiometry When More than One Reaction Occurs

A limestone analyses (weight %)

$CaCO_3$	92.89%
$MgCO_3$	5.41%
Inert	1.70%

By heating the limestone you recover oxides known as lime.

(a) How many pounds of calcium oxide can be made from 1 ton of this limestone?

(b) How many pounds of CO_2 can be recovered per pound of limestone?

(c) How many pounds of limestone are needed to make 1 ton of lime?

Solution:

The chemical reactions are:

$CaCO_3 \rightarrow CaO + CO_2$

$MgCO_3 \rightarrow MgO + CO_2$

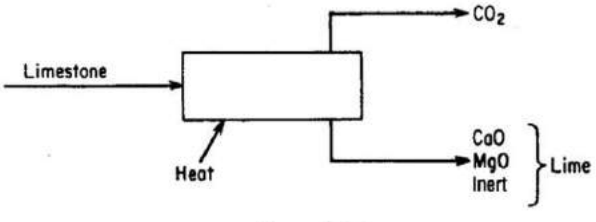


Figure E9.3

M.wt. of $CaCO_3$ = 100.1 Ib/Ibmol, $MgCO_3$ = 84.32 Ib/Ibmol, MgO = 40.32 Ib/Ibmol, CaO = 56.08 Ib/Ibmol and CO_2 = 44 Ib/Ibmol

Basis: 100 Ib of limestone

Limestone			Solid Products		
Component	lb = percent	lb mol	Compound	lb mol	lb
$CaCO_3$	92.89	0.9280	CaO	0.9280	52.04
$MgCO_3$	5.41	0.0642	MgO	0.0642	2.59
Inert	1.70		Inert		1.70
Total	100.00	0.9920	Total	0.9920	56.33

The quantities listed under Products are calculated from the chemical equations. For example, for the last column:

$$\frac{92.89 \text{ lb } CaCO_3}{} \left| \frac{1 \text{ lb mol } CaCO_3}{100.1 \text{ lb } CaCO_3} \right| \frac{1 \text{ lb mol CaO}}{1 \text{ lb mol } CaCO_3} \left| \frac{56.08 \text{ lb CaO}}{1 \text{ lb mol CaO}} \right. = 52.04 \text{ lb CaO}$$

$$\frac{5.41 \text{ lb } MgCO_3}{} \left| \frac{1 \text{ lb mol } MgCO_3}{84.32 \text{ lb } MgCO_3} \right| \frac{1 \text{ lb mol MgO}}{1 \text{ lb mol } MgCO_3} \left| \frac{40.32 \text{ lb MgO}}{1 \text{ lb mol MgO}} \right. = 2.59 \text{ lb MgO}$$

The production of CO_2 is:

0.9280 lb mol CaO is equivalent to 0.9280 lb mol CO_2
0.0642 lb mol MgO is equivalent to 0.0642 lb mol CO_2
Total 0.992 lb mol CO_2

$$\frac{0.992 \text{ lb mol } CO_2}{} \left| \frac{44.0 \text{ lb } CO_2}{1 \text{ lb mol } CO_2} \right. = 44.65 \text{ lb } CO_2$$

or Ib CO_2 = 100 - 56.33 = 44.65 Ib CO_2
1 ton = 2000 Ib

(a) $\text{CaO produced} = \frac{52.04 \text{ lb CaO}}{100 \text{ lb limestone}} \left| \frac{2000 \text{ lb}}{1 \text{ ton}} \right. = 1041 \text{ lb CaO/ton}$

(b) $CO_2 \text{ recovered} = \frac{43.65 \text{ lb } CO_2}{100 \text{ lb limestone}} = 0.437 \text{ lb } CO_2\text{/lb limestone}$

(c) $\text{Limestone required} = \frac{100 \text{ lb limestone}}{56.33 \text{ lb lime}} \left| \frac{2000 \text{ lb}}{1 \text{ ton}} \right. = \text{3550 lb limestone/ton lime}$

3. Limiting and Excess Reactants:

In most industrial processes, the quantities of reactants input are not in exact stoichiometric proportions as fixed by the reaction equation. It is generally desirable that some of the reacting materials be present in excess quantity over the amounts theoretically required for combination with other reactants.

a. The limiting reactant:

Is the species in a chemical reaction that would theoretically run out first (would be completely consumed) if the reaction were to proceed to completion according to the chemical equation and it has smallest **maximum extent of reaction**.

b. The excess reactant:

Is the reactant that is present in excess amount over the stoichiometric requirement equivalent to that of the limiting reactant and it has highest **maximum extent of reaction** that of the limiting reactant. If the reaction does not proceed to completion, all the reactants called excess reactants.

- **Percent excess:**

  It is the excess quantity of any reactant expressed as a percent of the stoichiometric amount theoretically required to react completely with the limiting reactant according to the chemical equation.

$$\% \text{ excess} = \left[\frac{\text{amount of the excess reactant feed} - \begin{array}{c}\text{amount of the excess reactant required}\\ \text{to react with the limiting reactant}\end{array}}{\begin{array}{c}\text{amount of the excess reactant required}\\ \text{to react with the limiting reactant}\end{array}}\right] \times 100$$

$$\% \text{ excess} = \left[\frac{\text{Feed} - \text{Theoritical amount required}}{\text{Theoritical amount required}}\right] \times 100$$

4. Extent of Reaction (ξ):

The extent of reaction is calculated by dividing the change in the number of moles of a species that occurs in a reaction, for either a reactant or a product, by the related stoichiometric coefficient.

$$\xi = \frac{n_i - n_{io}}{\nu_i}$$

where n_i = moles of species i present in the system after the reaction occurs

n_{io} = moles of species i present in the system when the reaction starts

ν_i = coefficient for species i in the particular chemical reaction equation (moles of species i produced or consumed per moles reacting)

ξ = extent of reaction (moles reacting)

Note:

The products of the reaction have positive signs and the reactants have negative signs

Example:

If 20 moles of CO are fed to a reactor with 10 moles of O_2 and form 15 moles of CO_2, calculate the extent of reaction?

$2CO + O_2 \rightarrow 2CO_2$

Solution:

The value of the change in the moles of CO_2 is: 15 — 0 = 15. The value of the stoichiometric coefficient for the CO_2 is 2 mol/mol reacting.

The extent of reaction (ξ) = $\frac{(15 - 0)\text{ mol } CO_2}{2\text{ mol } CO_2\text{/moles reacting}} = 7.5$ moles reacting

Example 9.4:

Determine the extent of reaction for the following chemical reaction:

$N_2 + 3H_2 \rightarrow 2NH_3$

given the following analysis of feed and product:

	Feed	Product
N_2	100 g	
H_2	50 g	
NH_3	5 g	90 g

Solution:

Based on NH_3:

$$n_i = \frac{90\ \text{g NH}_3}{}\left|\frac{1\ \text{g mol NH}_3}{17\ \text{g NH}_3}\right. = 5.294\ \text{g mol NH}_3$$

$$n_{i0} = \frac{5\ \text{g NH}_3}{}\left|\frac{1\ \text{g mole NH}_3}{17\ \text{g NH}_3}\right. = 0.294\ \text{g mol NH}_3$$

$$\xi = \frac{n_i - n_{i0}}{v_i} = \frac{(5.294 - 0.204)\text{g mol NH}_3}{2\ \text{g mol NH}_3/\text{moles reacting}} = 2.50\ \text{moles reacting}$$

Based on N_2:

$$n_i = 0$$

$$n_{i0} = \frac{100\ \text{g N}_2}{}\left|\frac{1\ \text{g mol N}_2}{28\ \text{g N}_2}\right. = 3.57\ \text{g mol N}_2$$

$$\xi = \frac{n_i - n_{i0}}{v_i} = \frac{(0 - 3.57)\ \text{g mol N}_2}{-1\ \text{g mol N}_2/\text{moles reacting}} = 3.57\ \text{moles reacting}$$

Based on H_2:

$$n_i = 0$$

$$n_{i0} = \frac{50\ \text{g H}_2}{}\left|\frac{1\ \text{g mol H}_2}{2\ \text{g H}_2}\right. = 25\ \text{g mol H}_2$$

$$\xi = \frac{n_i - n_{i0}}{v_i} = \frac{(0 - 25)\ \text{g mol N}_2}{-3\ \text{g mol N}_2/\text{moles reacting}} = 8.33\ \text{moles reacting}$$

Example 9.5:

If you feed 10 grams of N_2 gas and 10 grams of H_2 gas into a reactor:

a. What is the maximum number of grams of NH_3 that can be produced?
b. What is the limiting reactant?
c. What is the excess reactant?

Solution:

The chemical reaction is:

$N_2 + 3H_2 \rightarrow 2NH_3$

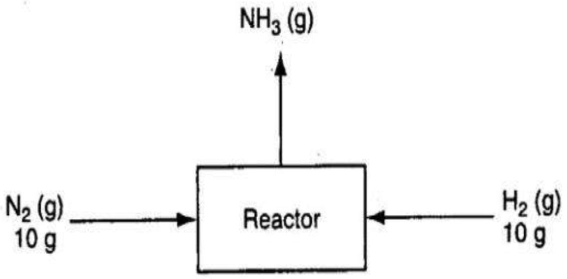


Figure E9.5

Next, write down the chemical equation, and get the molecular weights:

	$N_2(g)$	+	$3H_2(g)$	→	$2NH_3(g)$
Given g:	10		10		0
MW:	28		2.016		17.02
Calcd. g mol:	0.357		4.960		0

The next step is to determine the limiting reactant by calculating the max mum extent of reaction based on the complete reaction of N_2 and H_2.

$$\xi^{\max} \text{ (based on } N_2) = \frac{-0.357 \text{ g mol } N_2}{-1 \text{ g mol } N_2/\text{moles reacting}} = 0.357 \text{ moles reacting}$$

$$\xi^{\max} \text{ (based on } H_2) = \frac{-4.960 \text{ g mol } H_2}{-3 \text{ g mol } H_2/\text{moles reacting}} = 1.65 \text{ moles reacting}$$

You can conclude that N_2 is the limiting reactant and H_2 is the excess reactant:

$$\% \text{ excess } (H_2) = \left[\frac{4.960 - 3(0.357)}{3(0.357)}\right] \times 100 = 363.12\ \%$$

the maximum amount of NH_3 that can be produced is based on assuming complete conversion of the limiting reactant

$$\frac{0.357 \text{ g mol } N_2}{} \left| \frac{2 \text{ g mol } NH_3}{1 \text{ g mol } N_2} \right| \frac{17.02 \text{ g } NH_3}{1 \text{ g mol } NH_3} = 12.2 \text{ g } NH_3$$

5. Conversion and degree of completion

In spite of using excess amount of some reactants, many industrial reactions does not go to the completion, i.e. part of the limiting reactant is reacted and the other part remains unchanged.

a. Degree of completion:

Is the fraction of the *limiting reactant* that is actually reacted and converted into products.

$$\text{Fractional degree of completion} = \left[\frac{\text{moles (or mass) of the limiting reactant that react}}{\text{moles (or mass) of the limiting reactant that introduce (input)}}\right]$$

b. Conversion:

Is the fraction of the feed or some *key* material in the feed (usually the *excess reactant*) actually reacted and converted into products.

$$\%\ \text{Conversion} = \left[\frac{\text{moles (or mass) of feed (or a compound in the feed) that react}}{\text{moles (or mass) of feed (or a compound in the feed) that introduce (input)}}\right] \times 100$$

Note:

- The amount actually reacted is computed from the amount of product that is produced from the reaction.
- % conversion is dimensionless.

Example: For the reaction $C_7H_{16} + 11O_2 \rightarrow 7CO_2 + 8H_2O$

If 14.4 kg of CO_2 are formed in the reaction of 10 kg of C_7H_{16}, what is the percent of conversion of the C_7H_{16} to convert to CO_2?

Solution:

$$\begin{array}{c}\text{C}_7\text{H}_{16}\text{ equivalent}\\ \text{to CO}_2\text{ in the product}\end{array} = \frac{14.4\ \text{kg CO}_2}{}\left|\frac{1\ \text{kg mol CO}_2}{44.0\ \text{kg CO}_2}\right|\frac{1\ \text{kg mol C}_7\text{H}_{16}}{7\ \text{kg mol CO}_2} = 0.0468\ \text{kg mol C}_7\text{H}_{16}$$

$$\text{C}_7\text{H}_{16}\text{ in the reactants} = \frac{10\ \text{kg C}_7\text{H}_{16}}{}\left|\frac{1\ \text{kg mol C}_7\text{H}_{16}}{100.1\ \text{kg C}_7\text{H}_{16}}\right. = 0.0999\ \text{kg mol C}_7\text{H}_{16}$$

$$\%\ \text{conversion} = \frac{0.0468\ \text{mol reacted}}{0.0999\ \text{kg mol fed}}100 = 46.8\%\ \text{of the C}_7\text{H}_{16}$$

6. Selectivity:

Is the ratio of the moles of a particular (usually the *desired*) product to the moles of another (usually *undesired* or by-product) product produced in a set of reactions.

$$\text{Selectivity} = \left[\frac{\text{moles of desired product}}{\text{moles of undesired product}}\right]$$

Example: Methanol can be converted into ethylene (C_2H_4) or propylene (C_3H_6) by the reactions:

$2\ CH_3OH \rightarrow C_2H_4 + 2H_2O$ desired product (economical)
$3\ CH_3OH \rightarrow C_3H_6 + 3H_2O$ by-product

What is the selectivity of C_2H_4 relative to the C_3H_6 at 80% conversion of the CH_3OH?

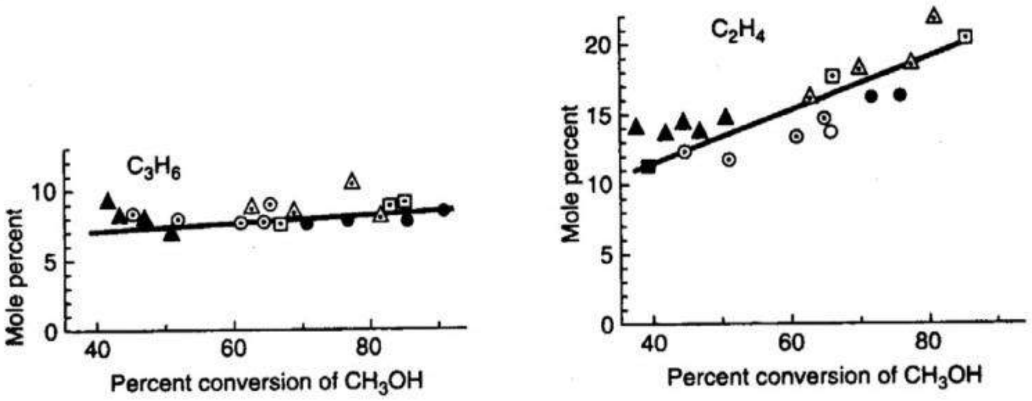


Figure 9.1 Products from the conversion of ethanol.

Solution:

From figure above,
at 80% conversion of CH_3OH to $C_2H_4 \approx 19$ mol%
at 80% conversion of CH_3OH to $C_3H_6 \approx 8$ mol%
Selectivity = (19/8) = 2.4 mol C_2H_4 per mol C_3H_6

7. Yield:

a. Yield (based on feed):

The amount (mass or moles) of desired product obtained divided by the amount of the key (frequently the limiting) reactant fed.

$$\text{Yield (based on feed)} = \left[\frac{\text{moles (or mass) of desired product}}{\text{moles (or mass) of limiting reactant fed (input)}}\right]$$

b. Yield (based on reactant consumed):

The amount (mass or moles) of desired product obtained divided by the amount of the key (frequently the limiting) reactant consumed.

$$\text{Yield (based on reactant consumed)} = \left[\frac{\text{moles (or mass) of desired product}}{\text{moles (or mass) of limiting reactant consumed(reacted)}}\right]$$

***It is important to know that incomplete reactions and side reactions reduce the yield.**

Example 9.8:

We have two reactions:

Cl_2 (g) + C_3H_6 (g) → C_3H_5Cl (g) + HCl ......…………….. (a)
Cl_2 (g) + C_3H_6 (g) → $C_3H_6Cl_2$ (g) …………………..(b)

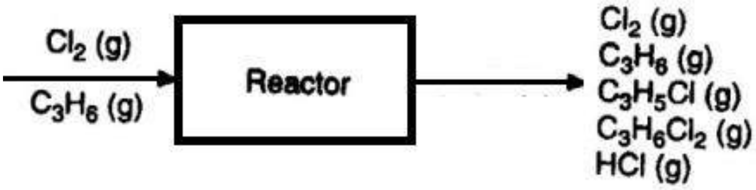
The species recovered after the reaction takes place for some time are listed in table below:

Species	MW	gmol
Cl_2		141.0
C_3H_6, propylene	42.08	651.0
C_3H_5Cl, ally chloride	76.53	4.6
$C_3H_6Cl_2$, propylene chloride	112.99	24.5
HCl		4.6

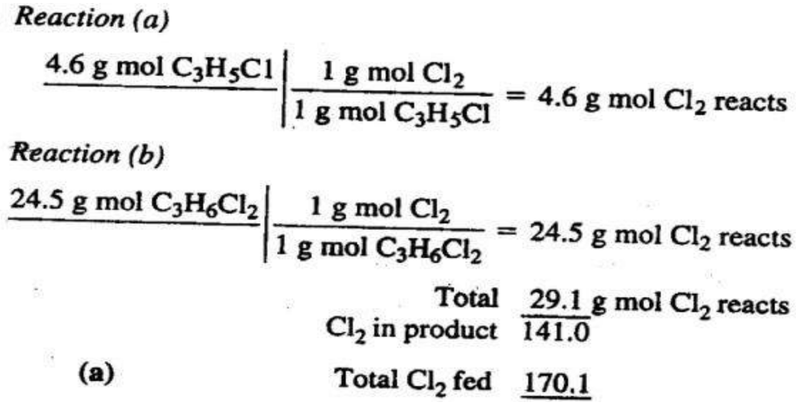
Based on the product distribution assuming that no ally chlorides were present in the feed, calculate the following:

a. How much $C1_2$ and C_3H_6 were fed to the reactor in gmol?
b. What was the limiting reactant?
c. What was the excess reactant?
d. What was the fraction conversion of C_3H_6 to C_3H_5C1?
e. What was the selectivity of C_3H_5C1 relative to $C_3H_6C1_2$?
f. What was the yield of C_3H_5CI expressed in g of C_3H_5C1 to the g of C_3H_6 fed to the reactor?
g. What was the extent of reaction of the first and second reactions?

Solution:



First calculate the gmol fed to the reactor (even if the amounts were not asked):



Reaction (a)

$$\frac{4.6 \text{ g mol } C_3H_5C1}{} \left| \frac{1 \text{ g mol } Cl_2}{1 \text{ g mol } C_3H_5Cl} \right. = 4.6 \text{ g mol } Cl_2 \text{ reacts}$$

Reaction (b)

$$\frac{24.5 \text{ g mol } C_3H_6Cl_2}{} \left| \frac{1 \text{ g mol } Cl_2}{1 \text{ g mol } C_3H_6Cl_2} \right. = 24.5 \text{ g mol } Cl_2 \text{ reacts}$$

Total 29.1 g mol Cl_2 reacts
Cl_2 in product 141.0

(a) Total Cl_2 fed 170.1

From the chemical equations you can see that if 29.1 gmol Cl_2 reacts by reaction (a) and (b), the same quantity of 29.1 gmol of C_3H_6 must react.

C_3H_6 in the product = 651.0 gmol
Total C_3H_6 fed = 651.0 + 29.1 = 680.1 gmol C_3H_6

(b) and (c) Since both reactions involve the same value of the respective reaction stoichiometric coefficients, both reactions will have the same limiting and excess reactants

$$\xi^{\max} \text{ (based on } C_3H_6) = \frac{-680.1 \text{ g mol } C_3H_6}{-1 \text{ g mol } C_3H_6\text{/moles reacting}} = 680.1 \text{ moles reacting}$$

$$\xi^{\max} \text{ (based on } Cl_2) = \frac{-170.1 \text{ g mole } Cl_2}{-1 \text{ g mol } Cl_2\text{/moles reacting}} = 170.1 \text{ moles reacting}$$

Thus, C_3H_6 was the excess reactant and Cl_2 the limiting reactant.

(d) The fraction conversion of C_3H_6 to C_3H_5Cl was

$$\frac{4.6 \text{ g mol } C_3H_6 \text{ that reacted}}{680.1 \text{ g mol } C_3H_6 \text{ fed}} = 6.76 \times 10^{-3}$$

(e) The selectivity was

$$\frac{4.6 \text{ g mol } C_3H_5Cl}{24.5 \text{ g mol } C_3H_6Cl_2} = 0.19 \frac{\text{g mol } C_3H_5Cl}{\text{g mol } C_3H_6Cl_2}$$

(f) The yield was

$$\frac{(76.53)(4.6)\text{g } C_3H_5Cl}{(42.08)(680.1)\text{g } C_3H_6} = 0.012 \frac{\text{g } C_3H_5Cl}{\text{g } C_3H_6}$$

(g) Because C_3H_5Cl is produced only by the first reaction, the extent of reaction of the first reaction is

$$\xi_1 = \frac{n_i - n_{io}}{v_i} = \frac{4.6 - 0}{1} = 4.6$$

Because $C_3H_6Cl_2$ is produced only by the second reaction, the extent of reaction of the second reaction is

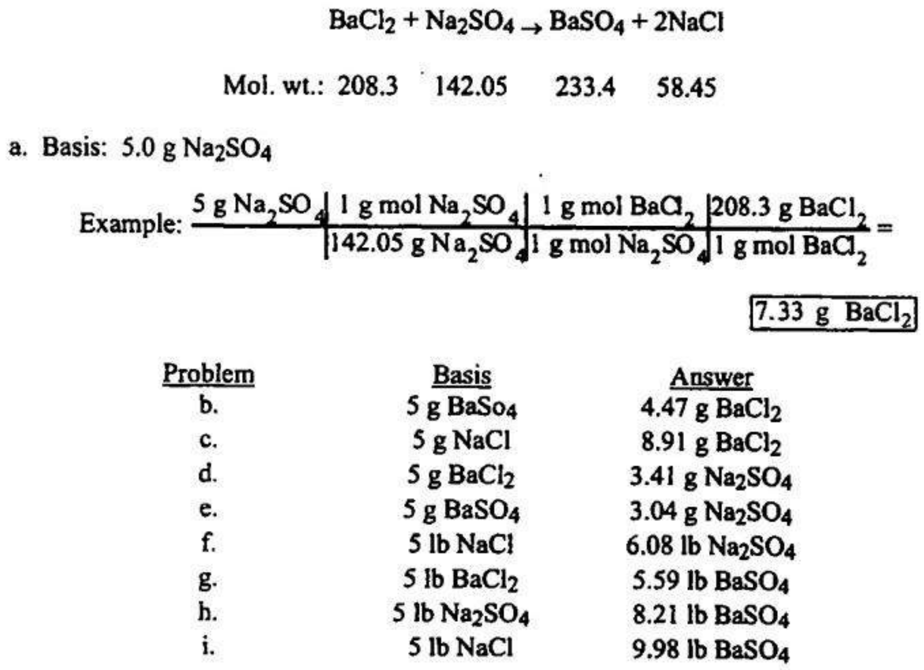
$$\xi_2 = \frac{n_i - n_{io}}{v_i} = \frac{24.5 - 0}{1} = 24.5$$

Problem 9.1:

$BaC1_2 + Na_2SO_4 \rightarrow BaSO_4 + 2NaC$

(a) How many grams of barium chloride will be required to react with 5.00 g of sodium sulfate?
(b) How many grams of barium chloride are required for the precipitation of 5.00 g of barium sulfate?
(c) How many grams of barium chloride are needed to produce 5.00 g of sodium chloride?
(d) How many grams of sodium sulfate are necessary for the precipitation of 5.00 g of barium chloride?
(e) How many grams of sodium sulfate have been added to barium chloride if 5.00 g of barium sulfate is precipitated?
(f) How many pounds of sodium sulfate are equivalent to 5.00 lb of sodium chloride?
(g) How many pounds of barium sulfate are precipitated by 5.00 lb of barium chloride?
(h) How many pounds of barium sulfate are precipitated by 5.00 lb of sodium sulfate?
(i) How many pounds of barium sulfate are equivalent to 5.00 lb of sodium chloride?

Solution:



$$BaCl_2 + Na_2SO_4 \rightarrow BaSO_4 + 2NaCl$$

Mol. wt.: 208.3 142.05 233.4 58.45

a. Basis: 5.0 g Na_2SO_4

$$\text{Example: } \frac{5\text{ g }Na_2SO_4}{} \left| \frac{1\text{ g mol }Na_2SO_4}{142.05\text{ g }Na_2SO_4} \right| \frac{1\text{ g mol }BaCl_2}{1\text{ g mol }Na_2SO_4} \left| \frac{208.3\text{ g }BaCl_2}{1\text{ g mol }BaCl_2} \right. =$$

$$\boxed{7.33\text{ g }BaCl_2}$$

Problem	Basis	Answer
b.	5 g $BaSo_4$	4.47 g $BaCl_2$
c.	5 g NaCl	8.91 g $BaCl_2$
d.	5 g $BaCl_2$	3.41 g Na_2SO_4
e.	5 g $BaSO_4$	3.04 g Na_2SO_4
f.	5 lb NaCl	6.08 lb Na_2SO_4
g.	5 lb $BaCl_2$	5.59 lb $BaSO_4$
h.	5 lb Na_2SO_4	8.21 lb $BaSO_4$
i.	5 lb NaCl	9.98 lb $BaSO_4$

Problem 9.23:

Antimony is obtained by heating pulverized stibnite (Sb_2S_3) with scrap iron and drawing off the molten antimony from the bottom of the reaction vessel.

$Sb_2S_3 + 3Fe \rightarrow 2Sb + 3FeS$

Suppose that 0.600 kg of stibnite and 0.250 kg of iron turnings are heated together to give 0.200 kg of Sb metal. Determine:

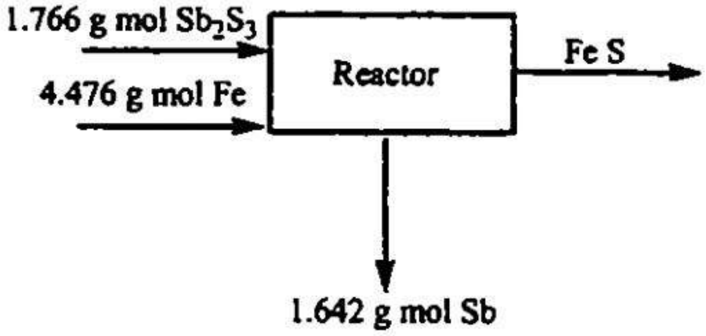
(a) The limiting reactant.
(b) The percentage of excess reactant.
(c) The degree of completion (fraction).
(d) The percent conversion based on Sb_2S_3.
(e) The yield in kg Sb produced/kg Sb_2S_3 fed to the reactor.

Solution:

The molecular weights needed to solve the problem and the gmol forming the basis are:

Component	kg	M.wt.	gmol
Sb_2S_3	0.600	339.7	1.766
Fe	0.250	55.85	4.476
Sb	0.200	121.8	1.642
FeS		87.91	

The process is illustrated as below:



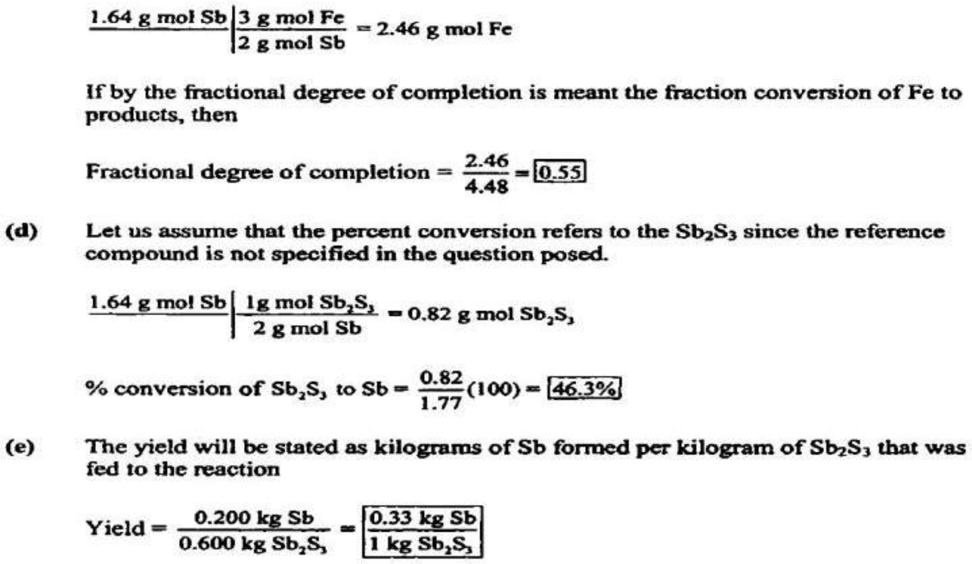
a. Moles of Sb_2S_3 = (0.6 x 1000) / 339.7 = 1.77 gmol
Moles of Fe = (0.25 x 1000) / 55.85 = 4.48 gmol

ξ^{max}(based on Sb_2S_3) = (-1.77/-1) = 1.776
ξ^{max}(based on Fe) = (-4.476/-3) = 1.492

Hence, the Fe is the limiting reactant and Sb_2S_3 is the excess reactant.
Theoretical Sb_2S_3 required to react with the limiting reactant = (4.476/3) = 1.492 gmol

b. $\%\text{ excess } = \left[\frac{1.776-1.492}{1.492}\right] = 18.4\ \%\text{ excess } Sb_2S_3$

c. Although Fe is the limiting reactant, not all the limiting reactant reacts. We can compute from the 1.64 gmol of Sb how much Fe actually does reacts:



$$\frac{1.64\text{ g mol Sb}}{}\left|\frac{3\text{ g mol Fe}}{2\text{ g mol Sb}}\right. = 2.46\text{ g mol Fe}$$

If by the fractional degree of completion is meant the fraction conversion of Fe to products, then

$$\text{Fractional degree of completion} = \frac{2.46}{4.48} = \boxed{0.55}$$

(d) Let us assume that the percent conversion refers to the Sb_2S_3 since the reference compound is not specified in the question posed.

$$\frac{1.64\text{ g mol Sb}}{}\left|\frac{1\text{g mol }Sb_2S_3}{2\text{ g mol Sb}}\right. = 0.82\text{ g mol }Sb_2S_3$$

$$\%\text{ conversion of }Sb_2S_3\text{ to Sb} = \frac{0.82}{1.77}(100) = \boxed{46.3\%}$$

(e) The yield will be stated as kilograms of Sb formed per kilogram of Sb_2S_3 that was fed to the reaction

$$\text{Yield} = \frac{0.200\text{ kg Sb}}{0.600\text{ kg }Sb_2S_3} = \boxed{\frac{0.33\text{ kg Sb}}{1\text{ kg }Sb_2S_3}}$$

Example 1.31:

Aluminum sulfate can be made by reacting crushed bauxite ore with sulfuric acid, according to the following equation:

$Al_2O_3 + 3H_2SO_4 \rightarrow Al_2(SO_4)_3 + 3H_20$

The bauxite ore contains 55.4% by weight of aluminum oxide, the remainder being impurities. The sulfuric acid solution contains 77.7% H_2SO_4, the rest being water.

To produce crude aluminum sulfate containing 1798 lb of pure aluminum sulfate, 1080 lb of bauxite ore and 2510 lb of sulfuric acid solution are used.

(a) Identify the excess reactant.
(b) What percentage of the excess reactant was consumed?
(c) What was the degree of completion of the reaction?

Solution:

Mass of Al_2O_3 input = (1080 x 0.554) = 598.32 Ib
$\Longrightarrow$ moles of Al_2O_3 input = (598.32/101.96) = 5.87 Ibmol
Mass of impurities input = (1080 x 0.4436) = 497.1 Ib = output of impurities
Mass of H_2SO_4 input = (2510 x 0.777) = 1950.27 Ib
$\Longrightarrow$ moles of H_2SO_4 input = (1950.27/98.1) = 19.88 Ibmol

ξ^{max}(based on Al_2O_3) = (-5.87/-1) = 5.87

ξ^{max}(based on H_2SO_4) = (-19.88/-3) = 6.63

Hence, the Al_2O_3 is the limiting reactant and H_2SO_4 is the excess reactant.
Theoretical Al_2O_3 required to react with the limiting reactant = (4.476/3) = 1.492 gmol

a. % excess $= \left[\frac{19.88-(5.87 \text{ x } 3)}{(5.87 \text{ x } 3)}\right] = 12.89\%$ excess H_2SO_4

b. Moles of $Al_2(SO_4)_3$ produced = (1798/342.2) = 5.25 Ibmol
The $Al_2(SO_4)_3$ actually formed indicates that:

$$\begin{array}{l|l} 5.25 \text{ lb mol } Al_2(SO_4)_3 & 3 \text{ lb mol } H_2SO_4 \\ \hline & 1 \text{ lb mol } Al_2(SO_4)_3 \end{array} = 15.75 \text{ lb mol } H_2SO_4 \text{ was consumed}$$

$$\frac{15.75}{19.88}(100) = 79.2\%$$

(c) The fractional degree of completion refers to the limiting reactant. For each mole of $Al_2(SO_4)_3$, 1 mole of Al_2O_3 was used:

$$\frac{5.25}{5.87} = 0.89$$

Example 1.32:

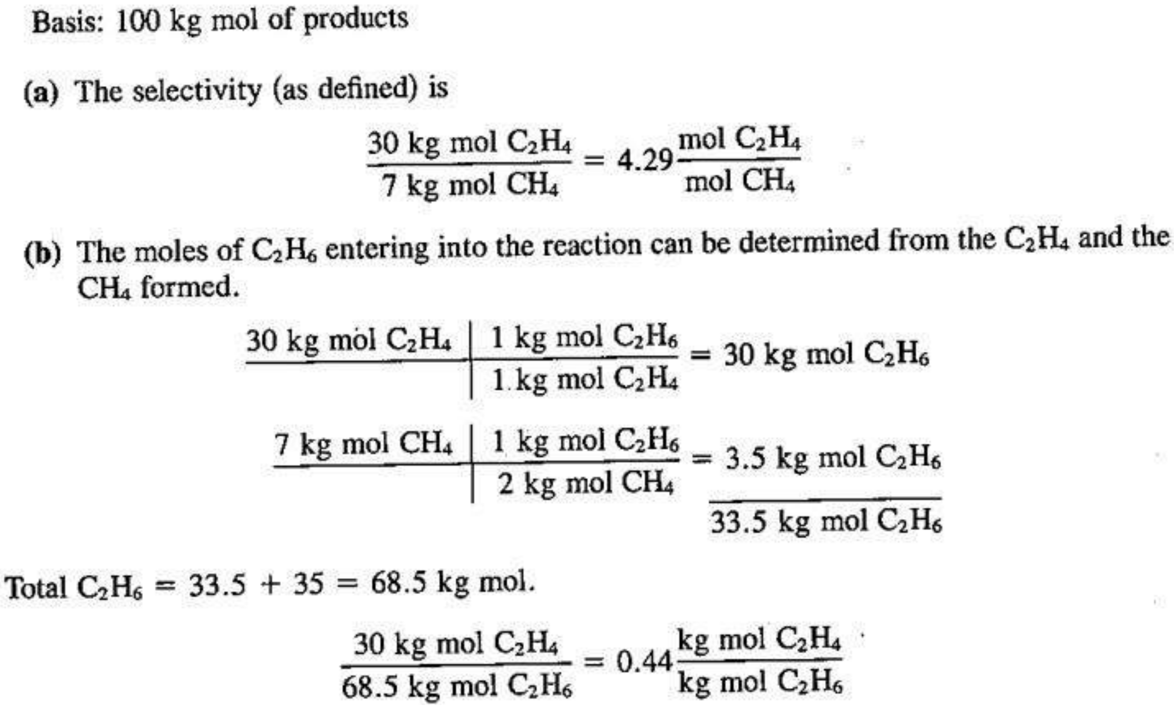
Ethylene (C_2H_4) can be produced by dehydration of ethane (C_2H_6). Methane can be produced as a by-product to the following reactions:

$C_2H_6 \rightarrow C_2H_4 + H_2$ ………………………..(1)
$C_2H_6 + H_2 \rightarrow 2CH_4$ ………………………..(2)
The composition (mol%) of the gases reaction product are given below:

Component	Percent
C_2H_6	35
C_2H_4	30
H_2	28
CH_4	7
Total	100

Calculate: (a) The selectivity of C_2H_4 relative to CH_4.
(b) The yield of C_2H_4 in kilogram moles of C_2H_4 per kilogram mole of C_2H_6.

Solution:



Basis: 100 kg mol of products

(a) The selectivity (as defined) is

$$\frac{30 \text{ kg mol } C_2H_4}{7 \text{ kg mol } CH_4} = 4.29 \frac{\text{mol } C_2H_4}{\text{mol } CH_4}$$

(b) The moles of C_2H_6 entering into the reaction can be determined from the C_2H_4 and the CH_4 formed.

$$\begin{array}{l|l} 30 \text{ kg mol } C_2H_4 & 1 \text{ kg mol } C_2H_6 \\ \hline & 1 \text{ kg mol } C_2H_4 \end{array} = 30 \text{ kg mol } C_2H_6$$

$$\begin{array}{l|l} 7 \text{ kg mol } CH_4 & 1 \text{ kg mol } C_2H_6 \\ \hline & 2 \text{ kg mol } CH_4 \end{array} = \frac{3.5 \text{ kg mol } C_2H_6}{33.5 \text{ kg mol } C_2H_6}$$

Total $C_2H_6 = 33.5 + 35 = 68.5$ kg mol.

$$\frac{30 \text{ kg mol } C_2H_4}{68.5 \text{ kg mol } C_2H_6} = 0.44 \frac{\text{kg mol } C_2H_4}{\text{kg mol } C_2H_6}$$

Chapter 10

Material Balances for Processes Involving Reaction

The general material balance for a process in which chemical reaction occurs is:

$$\left\{\begin{array}{c}\text{Accumulation}\\ \text{within the}\\ \text{system}\end{array}\right\} = \left\{\begin{array}{c}\text{Input}\\ \text{through}\\ \text{the system}\\ \text{boundaries}\end{array}\right\} - \left\{\begin{array}{c}\text{Output}\\ \text{through}\\ \text{the system}\\ \text{boundaries}\end{array}\right\} + \left\{\begin{array}{c}\text{Generation}\\ \text{within the}\\ \text{system}\end{array}\right\} - \left\{\begin{array}{c}\text{Consumption}\\ \text{within the}\\ \text{system}\end{array}\right\} \qquad (6.5)$$

Q: What terms of the general material balance, Equation (6.5), can be deleted if:

1. The process is known to be a steady state process.
2. The process is carried out inside a closed vessel.
3. The process does not involve a chemical reaction.

You might be given the value of the fraction conversion (f) of the limiting reactant; the extent of the reaction (ξ) is related to (f) by:

$$\xi = \frac{(-f)\, n^{\text{in}}_{\text{limiting reactant}}}{\nu_{\text{limiting reactant}}} \qquad \textbf{(10.5)}$$

Where:

$\nu_{\text{limiting reactant}}$: is the stoichiometric coefficient of the limiting reactant.

$n^{in}_{\text{limiting reactant}}$: is the no. of moles of the limiting reactant in the input stream.

f : is the fraction conversion of the limiting reactant.

ξ : is the extent of reaction

Example 10.1:

The chlorination of methane occurs by the following reaction

$CH_4 + Cl_2 \rightarrow CH_3C1 + HC1$

You are asked to determine the product composition if the conversion of the limiting reactant is 67%, and the feed composition in mole % is given as: 40% CH_4, 50% $C1_2$, and 10% N_2.

Solution:

Assume the reactor is an open, steady-state process. Figure E10.1 is a sketch of the process with the known information placed on it:

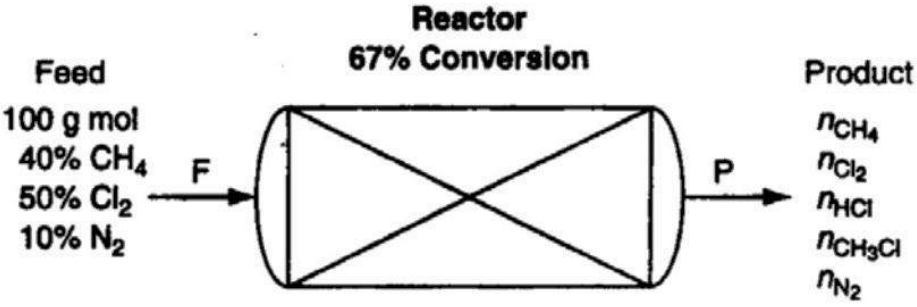


Figure E10.1

Select as a basis of 100 gmol feed.

$$\xi^{\max}(CH_4) = \frac{-n^{in}_{CH_4}}{\nu_{CH_4}} = \frac{-40}{(-1)} = 40$$

$$\xi^{\max}(Cl_2) = \frac{-n^{in}_{Cl_2}}{\nu_{Cl_2}} = \frac{-50}{(-1)} = 50$$

Therefore, CH_4 is the limiting reactant. You can now calculate the extent of the reaction using the specified conversion rate and Eq. (10.5)

$$\xi = \frac{(-f)\, n^{in}_{\text{limiting reactant}}}{\nu_{\text{limiting reactant}}} = \frac{(-0.67)(40)}{-1} = 26.8 \text{ gmoles reacting}$$

The species material balances (in moles) can be determined by using the calculated extent of reaction as below:

$$\xi = \frac{n_i^{\text{out}} - n_i^{\text{in}}}{\nu_i} \qquad i = 1, \cdots N$$

$$\boldsymbol{n}_{\mathbf{i}}^{\mathbf{out}} = \boldsymbol{n}_{\mathbf{i}}^{\mathbf{in}} + \xi\, \boldsymbol{\nu}_{\mathbf{i}}$$

$$\begin{aligned}
n_{CH_4}^{\text{out}} &= 40 - 1(26.8) = 13.2 \\
n_{Cl_2}^{\text{out}} &= 50 - 1(26.8) = 23.2 \\
n_{CH_3Cl}^{\text{out}} &= 0 + 1(26.8) = 26.8 \\
n_{HCl}^{\text{out}} &= 0 + 1(26.8) = 26.8 \\
n_{N_2}^{\text{out}} &= 10 - 0(26.8) = \underline{10.0} \\
&\qquad\qquad\qquad\; 100.0 = P
\end{aligned}$$

Therefore, the composition of the product stream is: 13.2% CH_4, 23.2% $C1_2$, 26.8% CH_3Cl, 26.8% HCI, and 10% N_2 because the total number of product moles is conveniently 100 g mol. There are 100 g mol of products because there are 100 g mol of feed and the chemical reaction equation results in the same number of moles for reactants as products.

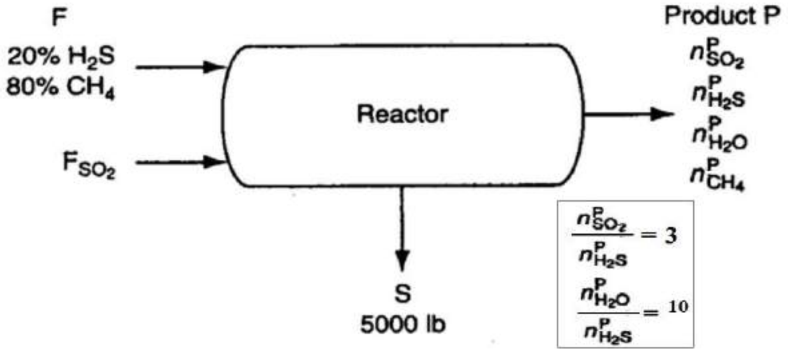
Example 10.2:

Hydrogen sulfide and other sulfur compounds are removed from natural gas by sweetening processes. As you know H_2S is toxic in very small quantities and is quite corrosive to process equipment. A proposed process to remove H_2S is by reaction with SO_2:

$2\,H_2S(g) + SO_2(g) \rightarrow 3S(s) + 2H_2O(g)$

In a test of the process, a gas stream containing 20% H_2S and 80% CH_4 was combined with a stream of pure SO_2. The process produced 5000 lb of S(s), and in the product gas the ratio of SO_2 to H_2S was equal to 3, and the ratio of H_2O to H_2S was 10. You are asked to determine the fractional conversion of the limiting reactant, and the feed rates of the H_2S and SO_2 streams.

Solution:



Basis: 5000 Ib of **S** =156.3 Ibmol of **S**

$$\boxed{\boldsymbol{n}_{\mathbf{i}}^{\mathbf{out}} = \boldsymbol{n}_{\mathbf{i}}^{\mathbf{in}} + \xi\, \boldsymbol{\nu}_{\mathbf{i}}}$$

The species balances in pound moles after introduction of most of the specifications are:

$$\text{S:} \quad 156.3 = 0 + 3\,\xi \tag{a}$$

$$\text{H}_2\text{S:} \quad n^P_{\text{H}_2\text{S}} = 0.20F - 2\,\xi \tag{b}$$

$$\text{SO}_2\text{:} \quad n^P_{\text{SO}_2} = F_{\text{SO}_2} - 1\,\xi \tag{c}$$

$$\text{H}_2\text{O:} \quad n^P_{\text{H}_2\text{O}} = 0 + 2\,\xi \tag{d}$$

$$\text{CH}_4\text{:} \quad n^P_{\text{CH}_4} = 0.80F + 0\,(\xi) \tag{e}$$

The remaining specifications are

$$n^P_{\text{SO}_2} = 3n^P_{\text{H}_2\text{S}} \tag{f}$$

$$n^P_{\text{H}_2\text{O}} = 10n^P_{\text{H}_2\text{S}} \tag{g}$$

Equations (a) through (g) comprise seven independent equations and seven unknowns:

If you solve the equations without using a computer, you should start by calculating ξ from Equation (a)

$$\xi = \frac{156.3 \text{ mol}}{3} = 52.1 \text{ mol rxn}$$

Then Equation (d) gives

$$n^P_{H_2O} = 2(52.1) = 104.2 \text{ lb mol } H_2O$$

Next, Equation (g) gives

$$n^P_{H_2S} = \frac{1}{10} n^P_{H_2O} = 10.4 \text{ lb mol } H_2S$$

and Equation (f) gives

$$n^P_{SO_2} = 3(10.4) = 31.2 \text{ lb mol } SO_2$$

If you solve the rest of the equations in the order (b), (c), and (e), you find

$$F = 573 \text{ lb mol}$$
$$F_{SO_2} = 83.3 \text{ lb mol}$$
$$n^F_{CH_4} = 458 \text{ lb mol}$$

Finally, you can identify H_2S as the limiting reactant because the molar ratio of SO_2 to H_2S in the product gas (3/1) is greater than the molar ratio in the chemical reaction equation (2/1). The fractional conversion from Equation (10.5) is the consumption of H_2S divided by the total feed of H_2S

$$f = \frac{-(-2)\xi}{0.2F} = \frac{(2)(52.1)}{(0.2)(573)} = 0.91$$

Explain:

$$\xi_{H_2S} = \frac{n_i - n_{io}}{\nu_i} = \frac{10.4 - [(0.2)(573)]}{-2} = 52.1$$

$$\xi_{SO_2} = \frac{n_i - n_{io}}{\nu_i} = \frac{31.2 - 83.3}{-1} = 52.1$$

	in	out
SO_2	83.3	31.2
H_2S	114.6	10.4

$$\frac{n^p_{SO_2}}{n^p_{H_2S}} = \frac{31.2}{10.4} = 3$$

Example : A gaseous mixture consists of 80 mol% N_2 and 20 mol% CO_2 are continuously fed to the absorber column in which CO_2 are completely absorbed by sodium hydroxide solution according to the following reaction:

	CO_2 +	2NaOH →	Na_2CO_3 +	H_2O
M.wt	44	40	106	18

The product liquid stream are left the bottom of the absorber at a rate of 1000 Ib/hr with composition of 26.5 wt.% Na_2CO_3, 4 wt.% NaOH and 69.5 wt.% H_2O. Pure nitrogen are out from top of the column. Calculate:

a. The mass flow rate and composition (wt.%) of NaOH solution.
b. The mass flow rates of input and output gaseous streams.
c. % excess and conversion of NaOH.

Solution:

(a) Basis: 1000 Ib of product solution

Mass of Na_2CO_3 produced = (1000) (0.265) = 265 Ib
Moles of Na_2CO_3 produced = (265/106) = 2.5 Ibmole

Moles of NaOH reacted = (2.5) (2/1) = 5 Ibmole
Mass of NaOH reacted = (5) (40) = 200 Ib
Mass of NaOH output = (1000) (0.04) = 40 Ib
Mass of NaOH input = Reacted + output = 200 + 40 = 240 Ib

Moles of H_2O produced from reaction = (2.5) (1/1) = 2.5 Ibmole
Mass of H_2O produced from reaction = (2.5) (18) = 45 Ib
Mass of H_2O output = (1000) (0.695) = 695 Ib
Mass of H_2O input = output – produced = 695 – 45 = 650 Ib

Mass of NaOH solution input = 240 + 650 = 890 Ib/hr

(b) Moles of CO_2 reacted = (2.5) (1/1) = 2.5 Ibmole

Since CO_2 are completely reacted

Moles of N_2 input = (2.5) (80/20) = 10 Ibmole
The flow rate of feed gas = (2.5) (44) + (10) (28) = 390 Ib/hr
The flow rate of exit gas = (10) (28) = 280 Ib/hr

Checking: Input = 890 + 390 = 1280 Ib/hr
Output = 1000 + 280 = 1280 Ib/hr

(c) Moles of NaOH reacted = 5 Ibmole
Mass of NaOH input = 240 Ib
Moles of NaOH input = (240/40) = 6 Ibmole

% excess of NaOH = ((6 – 5) /5) *100 =20%
% conversion of NaOH = (5/6)*100 = 83.3 %

Example : Hydrofluoric acid can be manufactured by treating crushed fluorspar ore with an excess amount of sulfuric acid solution according to the reaction:

$$CaF_2 + H_2SO_4 \rightarrow CaSO_4 + 2HF$$

M.wt. 78 98 136 20

The fluorspar ore (F) contains 78 wt.% CaF_2 and 22 wt.% inert impurities. The acid solution (S) contains 95 wt.% H_2SO_4. The reaction goes to completion and all HF and water are volatilized and sepdarated as vapour (V) from residual sulfate cake (R) which contains 16 wt.% H_2SO_4. On the basis of 1000 Ib of the fluorspar charged, calculate:

(a) The quantities of S, V, R and the composition of (V) and (R).
(b) % excess of H_2SO_4.

Solution:

(a) Basis: 1000 Ib of (F)

Mass of CaF_2 input = (1000) (0.78) = 780 Ib
Moles of CaF_2 input = (780/78) = 10 Ibmole = quantity reacted since the reacting goes to completion
Mass of impurities input = 220 Ib = quantity output in (R)
Moles of $CaSO_4$ produced = (10) (1/1) = 10 Ibmole
Mass of $CaSO_4$ produced = (10) (136) = 1360 Ib
Mass of $CaSO_4$ produced + Mass of impurities input = 1360 + 220 = **1580 Ib = (R) (0.84)**
⟹ R= 1881 Ib
Mass of H_2SO_4 in (R) = (1881) (0.16) = 301 Ib

Mass of H_2SO_4 input = H_2SO_4 reacted + H_2SO_4 unreacted (output)
=(10) (98) + 301 = **1281 Ib = (S) (0.95)**
⟹ S= 1348 Ib
Mass of water input = Mass of water output (V) = (1348) (0.05) = 67 Ib

Moles of HF produced = (10) (2/1) = 20 Ibmole
Mass of HF produced = (20) (20) = 400 Ib
Vapour (V) = 400 + 67 = 467 Ib

Checking: Input = F + S = 1000 + 1348 = 2348 Ib
Output = R + V = 1881 + 467 = 2348 Ib

(b) Mass of H_2SO_4 input = 1281 Ib
Moles of H_2SO_4 input = (1281/98) = 13.07 Ibmole
Moles of H_2SO_4 reacted = 10 Ibmole
% excess of H_2SO_4 = ((13.07-10)/10)*100 = 30.7%

Processes Involving Multiple Reactions

In practice reaction systems rarely involve just a single reaction. A primary reaction (e.g., the desired reaction) can occur, but there are always additional or side reactions. To extend the concept of the extent of reaction to processes involving multiple reactions, the question is do you just include a ξ for every reaction. The answer is no. You should include in the species material balances only the ξ i associated with a (nonunique) set of independent chemical reactions called the minimal set of reaction equations. What this term means is the smallest set of chemical reactions equations that can be assembled that includes all of the species involved in the process. Analogous to a set of independent linear algebraic equations, you can form any other reaction equation by a linear combination of the reaction equations contained in the minimal set. For example, look at the following set of reaction equations:

$C + O_2 \rightarrow CO_2$ ……………………...(1)
$C + 1/2\ O_2 \rightarrow CO$ ……………………..(2)
$CO + 1/2\ O_2 \rightarrow CO_2$ …………………..(3)

By inspection you can see that if you subtract the second equation from the first one, you obtain the third equation. Only two of the three equations are independent, hence the minimal set is comprised of any two of the three equations.

For open, steady state processes with multiple reactions, Equation (6.5) in moles becomes for component i:

$$n_i^{\text{out}} = n_i^{\text{in}} + \sum_{j=1}^{R} \nu_{ij}\,\xi_j \tag{10.6}$$

where

ν_{ij} is the stoichiometric coefficient of species i in reaction j in the minimal set.

ξ_j is the extent of reaction for the jth reaction in the minimal set.

R is the number of independent chemical reaction equations (the size of the minimal set).

For a closed, unsteady state system:

The total moles (N) exiting a reactor are:

$$N = \sum_{i=1}^{S} n_i^{\text{out}} = \sum_{i=1}^{S} n_i^{\text{in}} + \sum_{i=1}^{S}\sum_{j=1}^{R} \nu_{ij}\xi_j \tag{10.7}$$

Where: **S** is the number of species in the system:

Example 10.3: Material Balances for a Process in Which Two Simultaneous Reactions Occurs

Formaldehyde (CH_2O) is produced industrially by the catalytic oxidation of methanol (CH_3OH) according to the following reaction:

$CH_3OH + 1/2\ O_2 \rightarrow CH_2O + H_2O$ ……………………………………….. (1)

Unfortunately, under the conditions used to produce formaldehyde at a profitable rate, a significant portion of the formaldehyde reacts with oxygen to produce CO and H_2O, that is,

$CH_2O + 1/2\ O_2 \rightarrow CO + H_2O$ ………………………………………………(2)

Assume that methanol and twice the stoichiometric amount of air needed for complete conversion of the CH_3OH to the desired products (CH_2O and H_2O) are fed to the reactor. Also assume that 90% conversion of the methanol results, and that a 75% yield of formaldehyde occurs based on the theoretical production of CH_2O by Reaction 1. Determine the composition of the product gas leaving the reactor.

Solution:

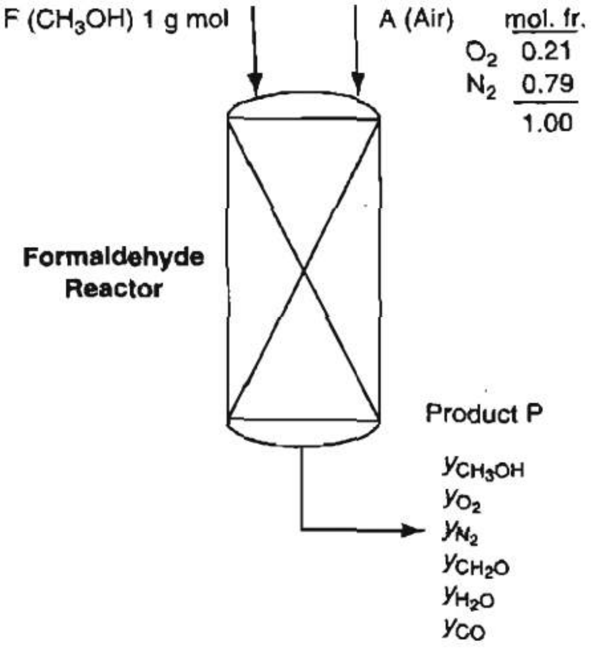


Figure E10.3

Basis: 1 gmol of **F**

Let:

ξ_1 represent the extent of reaction for the first reaction (1).

ξ_2 represent the extent of reaction for the second reaction (2).

The limiting reactant is CH_3OH.

$$\xi_1 = \frac{(-f)\, n^{\text{in}}_{\text{limiting reactant}}}{\nu_{\text{limiting reactant}}} \qquad = \frac{(-0.9)(1)}{-1} = 0.9 \text{ gmoles reacting}$$

The yield is related to ξ as follows:

By reaction (1): $n^{\text{out},1}_{CH_2O} = n^{\text{in},1}_{CH_2O} + (\nu_{CH_2O})(\xi_1) = 0 + (1)(\xi_1)$

$$n^{\text{out},1}_{CH_2O} = \xi_1$$

By reaction (2): $n^{\text{out},2}_{CH_2O} = n^{\text{in},2}_{CH_2O} + (\nu_{CH_2O})(\xi_2)$

But: $\boxed{n^{\text{in},2}_{CH_2O} = n^{\text{out},1}_{CH_2O}}$

$$n^{\text{out},2}_{CH_2O} = (\xi_1) + (-1)(\xi_2)$$

$$n^{\text{out},2}_{CH_2O} = \xi_1 - \xi_2$$

$$\text{The yield} = \frac{\text{Desired product}}{\text{limiting reactant}} = \frac{n^{\text{out},2}_{CH_2O}}{F} = \frac{\xi_1 - \xi_2}{1} = 0.75$$

$$0.75 = \frac{0.9 - \xi_2}{1}$$

$$\Longrightarrow \quad \xi_2 = 0.15 \text{ gmoles reacting}$$

You should next calculate the amount of air (A) that enters the process. The entering oxygen is twice the required oxygen based on reaction (1):

$$n^{A}_{O_2} = 2\left(\frac{1}{2}\ F\right) = 2\left(\frac{1}{2}\right)(1.0) = 1.0 \text{ gmol}$$

$$A = \frac{n^{A}_{O_2}}{0.21} = \frac{1.0}{0.21} = 4.76 \text{ gmol}$$

$$n^{A}_{N_2} = 4.76 - 1.0 = 3.76 \text{ gmol}$$

Species material balances = 6 = [CH_3OH, O_2, N_2, CH_2O, H_2O, CO]

Let us calculate **P** using Eq.(10.7)

$$P = \sum_{i=1}^{S} n_i^{in} + \sum_{i=1}^{S}\sum_{j=1}^{R} v_{i_j}\,\xi_j$$

$$= 1 + 4.76 + \sum_{i=1}^{6}\sum_{j=1}^{2} v_{i_j}\,\xi_j$$

$$= 5.76 + [(-1) + (-1/2) + (1) + 0 + (1) + 0]\,0.9$$

$$+ [0 + (-1/2) + (-1) + 0 + (1) + (1)]\,0.15 = 6.28 \text{ g mol}$$

P = 6.28 gmol

The material balances using Eq.(10.6):

$$n_i^{\text{out}} = n_i^{\text{in}} + \sum_{j=1}^{R} \nu_{ij}\,\xi_j \qquad (10.6)$$

$$n_{\text{CH}_3\text{OH}}^{\text{out}} = y_{\text{CH}_3\text{OH}}\,(6.28) = 1 - (0.9) + 0 = 0.10$$

$$n_{\text{O}_2}^{\text{out}} = y_{\text{O}_2}\,(6.28) = 1.0 - (1/2)(0.9) - (1/2)(0.15) = 0.475$$

$$n_{\text{CH}_2\text{O}}^{\text{out}} = y_{\text{CH}_2\text{O}}\,(6.28) = 0 + 1\,(0.9) - 1\,(0.15) = 0.75$$

$$n_{\text{H}_2\text{O}}^{\text{out}} = y_{\text{H}_2\text{O}}\,(6.28) = 0 + 1\,(0.9) + 1\,(0.15) = 1.05$$

$$n_{\text{CO}}^{\text{out}} = y_{\text{CO}}\,(6.28) = 0 + 0 + 1\,(0.15) = 0.15$$

$$n_{\text{N}_2}^{\text{out}} = y_{\text{N}_2}\,(6.28) = 3.76 - 0 - 0 = 3.76$$

You can check the value of P by adding all of the n_i^{out} above:
P = 0.1 + 0.475 + 0.75 + 1.05 + 0.15 + 3.76 = 6.28 gmol

The six equations can be solved for the y_i.:

$$y_{\text{CH}_3\text{OH}} = 1.6\%, \quad y_{\text{O}_2} = 7.6\%, \quad y_{\text{N}_2} = 59.8\%,$$

$$y_{\text{CH}_2\text{O}} = 11.9\%, \quad y_{\text{H}_2\text{O}} = 16.7\%, \quad y_{CO} = 2.4\%.$$

Example 10.4: Analysis of a Bioreactor

A bioreactor is a vessel in which biological conversion is carried out involving enzymes, microorganisms, and/or animal and plant cells. In the anaerobic fermentation of grain, the yeast Saccharomyces cerevisiae digests glucose ($C_6H_{12}O_6$) from plants to form the products ethanol (C_2H_5OH) and propenoic acid ($C_2H_3CO_2H$) by the following overall reactions:

$C_6H_{12}O_6 \rightarrow 2\,C_2H_5OH + 2CO_2$ ……………………………………….. (1)
$C_6H_{12}O_6 \rightarrow 2\,C_2H_3CO_2H + 2\,H_2O$ ……………………………...……... (2)

In a batch process, a tank is charged with 4000 kg of a 12% solution of glucose in water. After fermentation, 120 kg of CO_2 are produced and 90 kg of unreacted glucose remains in the broth. What are the weight (mass) percents of ethanol and propenoic acid in the broth at the end of the fermentation process? Assume that none of the glucose is assimilated into the bacteria.

Solution:

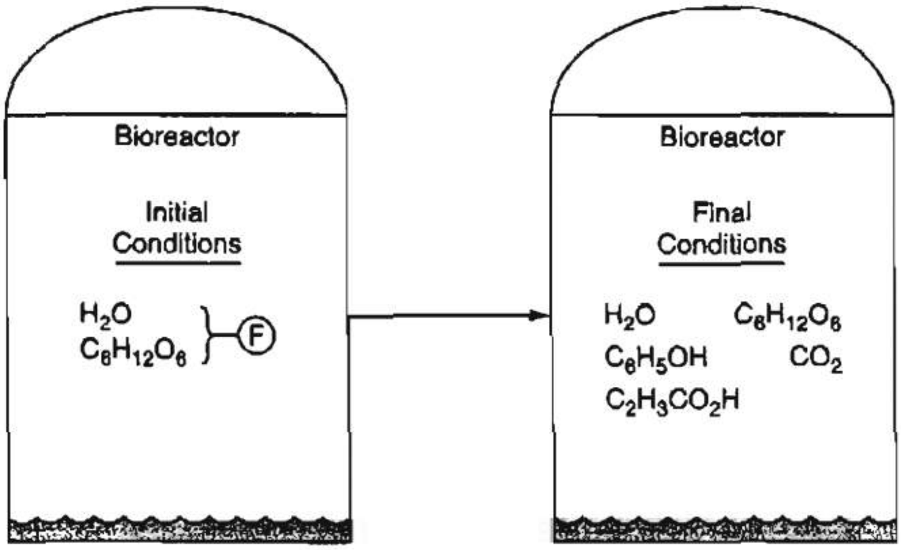


Figure E10.4

Basis: 4000 kg of **F**

$$n_i^{final} = n_i^{initial} + \sum_{j=1}^{R} v_{ij}\,\xi_j$$

You should convert the 4000 kg into moles of H_2O and $C_6H_{12}O_6$.

$$n_{H_2O}^{intial} = \frac{4000\ (0.88)}{18.02} = 195.3\ \text{kgmol}$$

$$n_{C_6H_{12}O_6}^{intial} = \frac{4000\ (0.12)}{180.1} = 2.665\ \text{kgmol}$$

Number of variables: 7

$$n_{H_2O}^{Final},\ n_{C_6H_{12}O_6}^{Final},\ n_{C_2H_5OH}^{Final},\ n_{C_2H_3CO_2H}^{Final},\ n_{CO_2}^{Final},\ \xi_1,\ \xi_2$$

$$n_{C_6H_{12}O_6}^{final} = \frac{90}{180.1} = 0.5\ \text{kgmol}$$

$$n_{CO_2}^{final} = \frac{120}{44} = 2.727\ \text{kgmol}$$

$$H_2O: \quad n_{H_2O}^{Final} = 195.3 + (0)\xi_1 + (2)\xi_2 \qquad \text{(a)}$$

$$C_6H_{12}O_6: \quad 0.500 = 2.665 + (-1)\xi_1 + (-1)\xi_2 \qquad \text{(b)}$$

$$C_2H_5OH: \quad n_{C_2H_5OH}^{Final} = 0 + 2\xi_1 + (0)\xi_2 \qquad \text{(c)}$$

$$C_2H_3CO_2H: \quad n_{C_2H_3CO_2H}^{Final} = 0 + (0)\xi_1 + (2)\xi_2 \qquad \text{(d)}$$

$$CO_2\ 2.727 = 0 + (2)\ \xi_1 + (0)\xi_2 \qquad \text{(e)}$$

The solution of Equations (a) – (e) is

ξ_1 = 1.364 kg moles reacting ξ_2 = 0.801 kg moles reacting

	Results	*Conversion to mass percent*		
Species	*kg kmol*	*MW*	*kg*	*Mass %*
H_2O	196.9	18.01	3546.1	88.7
C_2H_5OH	2.728	46.05	125.6	3.1
$C_2H_3CO_2H$	1.602	72.03	115.4	2.9
CO_2	2.277	44.0	120.0	3.0
$C_6H_{12}O_6$	0.500	180.1	90.1	2.3
			3997	1.00

The total mass of 3977 kg is close enough to 4000 kg of feed to validate the results of the calculations.

Element Material Balance

Elements in a process are conserved, and consequently you can apply **Equation (10.1)** to the elements in a process. Because elements are not generated or consumed, the generation and consumption terms in **Equation (10.1)** can be ignored. Element balances are especially useful when you do not know what reactions occur in a process. You only know information about the input and output stream components.

Example 10.1: Element balances

The chlorination of methane occurs by the following reaction

$CH_4 + Cl_2 \rightarrow CH_3C1 + HC1$

You are asked to determine the product composition if the conversion of the limiting reactant is 67%, and the feed composition in mole % is given as: 40% CH_4, 50% $C1_2$, and 10% N_2.

Solution:

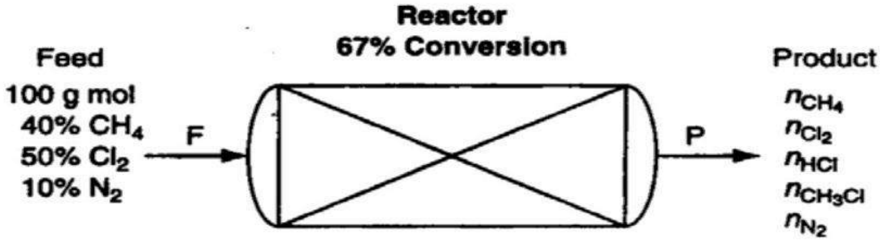


Figure E10.1

Select as a basis of 100 gmol feed.

Element balances: 4

C, H, Cl, N

Input = Output

$$\text{C:}\quad 100\,(0.40) = n^{\text{out}}_{CH_4}(1) + n^{\text{out}}_{CH_3Cl}(1)$$

$$\text{H:}\quad 100\,(0.40)(4) = n^{\text{out}}_{CH_4}(4) + n^{\text{out}}_{HCl}(1) + n^{\text{out}}_{CH_3Cl}(3)$$

$$\text{Cl:}\quad 100\,(0.50)(2) = n^{\text{out}}_{Cl_2}(2) + n^{\text{out}}_{HCl}(1) + n^{\text{out}}_{CH_3Cl}(1)$$

$$\text{2N:}\quad 100\,(0.10)(1) = n^{\text{out}}_{N_2}(1)$$

Substitute these equations for the species balances used in Example 10.1. As expected, the solution of the problem will be the same as found in Example 10.1.

Example 10.3: Element balances

Formaldehyde (CH_2O) is produced industrially by the catalytic oxidation of methanol (CH_3OH) according to the following reaction:

$CH_3OH + 1/2\ O_2 \rightarrow CH_2O + H_2O$ ……………………………………….. (1)

Unfortunately, under the conditions used to produce formaldehyde at a profitable rate, a significant portion of the formaldehyde reacts with oxygen to produce CO and H_2O, that is,

$CH_2O + 1/2\ O_2 \rightarrow CO + H_2O$ ………………………………………………(2)

Assume that methanol and twice the stoichiometric amount of air needed for complete conversion of the CH_3OH to the desired products (CH_2O and H_2O) are fed to the reactor. Also assume that 90% conversion of the methanol results, and that a 75% yield of formaldehyde occurs based on the theoretical production of CH_2O by Reaction 1. Determine the composition of the product gas leaving the reactor.

Solution:

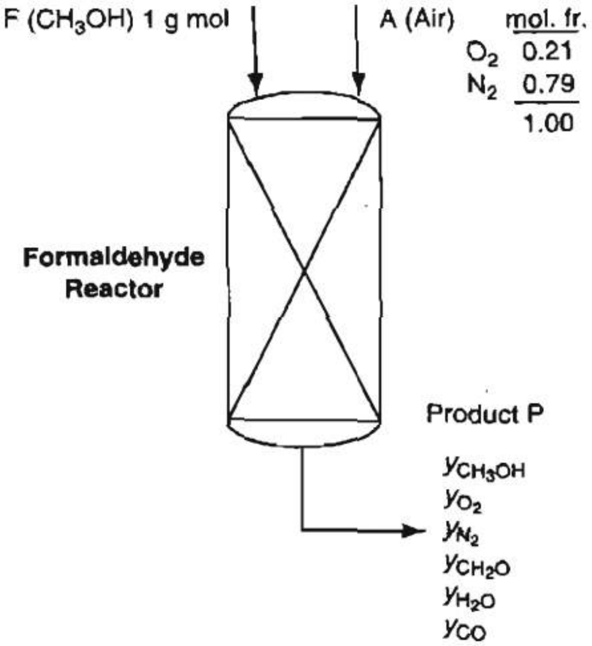


Figure E10.3

Basis: 1 gmol of **F**

Element balances: 4

C, H, O, N

$$\text{C:}\quad 1(1) + 4.76(0) = P[y^P_{CH_3OH}(1) + y^P_{CH_2O}(1) + y^P_{CO}(1)]$$

$$\text{H:}\quad 1(4) + 4.76(0) = P[y^P_{CH_3OH}(4) + y^P_{CH_2O}(2) + y^P_{H_2O}(2)]$$

$$\text{O:}\quad 1(1) + 1.00(2) = P[y^P_{CH_3OH}(1) + y^P_{O_2}(2) + y^P_{CH_2O}(1) + y^P_{H_2O}(1) + y^P_{CO}(1)]$$

$$\text{2N:}\quad 1(0) + 3.76 = P[y^P_{N_2}(1)]$$

Substitute these equations for the species balances used in Example 10.3. The solution of the problem will not change.

It would be easier to use the term $y_i^P P = n_i^P$ in the equations above in place of the product of two variables, y_i^P and P.

Example 10.6: Use of Element balances to Solve a Hydrocracking Problem

Hydrocracking is an important refinery process for converting low-valued heavy hydrocarbons into more valuable lower molecular weight hydrocarbons by exposing the feed to a zeolite catalyst at high temperature and pressure in the presence of hydrogen. Researchers in this field study the hydrocracking of pure components, such as octane (C_8H_{18}), to understand the behavior of cracking reactions. In one such experiment for the hydrocracking of octane, the cracked products had the following composition in mole percent: 19.5% C_3H_8, 59.4% C_4H_{10}, and 21.1% C_5H_{12}. You are asked to determine the molar ratio of hydrogen consumed to octane reacted for this process.

Solution:

We will use the element balances because the reactions in the process are not specified.

Basis: P =100 gmol

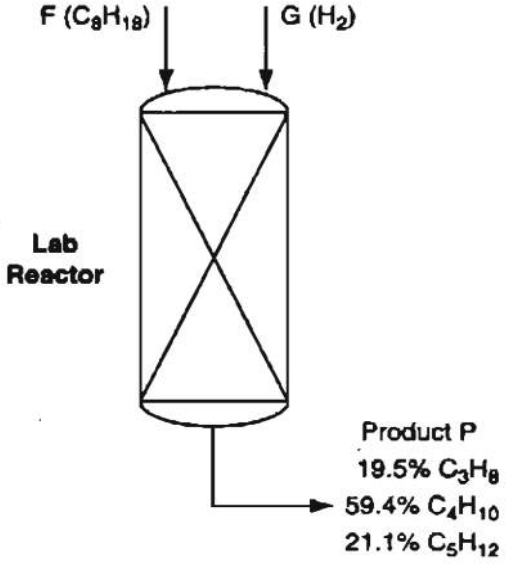


Figure E10.6

C: $F(8) + G(0) = 100[(0.195)(3) + (0.594)(4) + (0.211)(5)]$

H: $F(18) + G(2) = 100[(0.195)(8) + (0.594)(10) + (0.211)(12)]$

and the solution is

$$F = 50.2 \text{ g mol} \qquad G = 49.8 \text{ g mol}$$

The ratio

$$\frac{H_2 \text{ consumed}}{C_8H_{18} \text{ reacted}} = \frac{49.8 \text{ g mol}}{50.2 \text{ g mol}} = 0.992$$

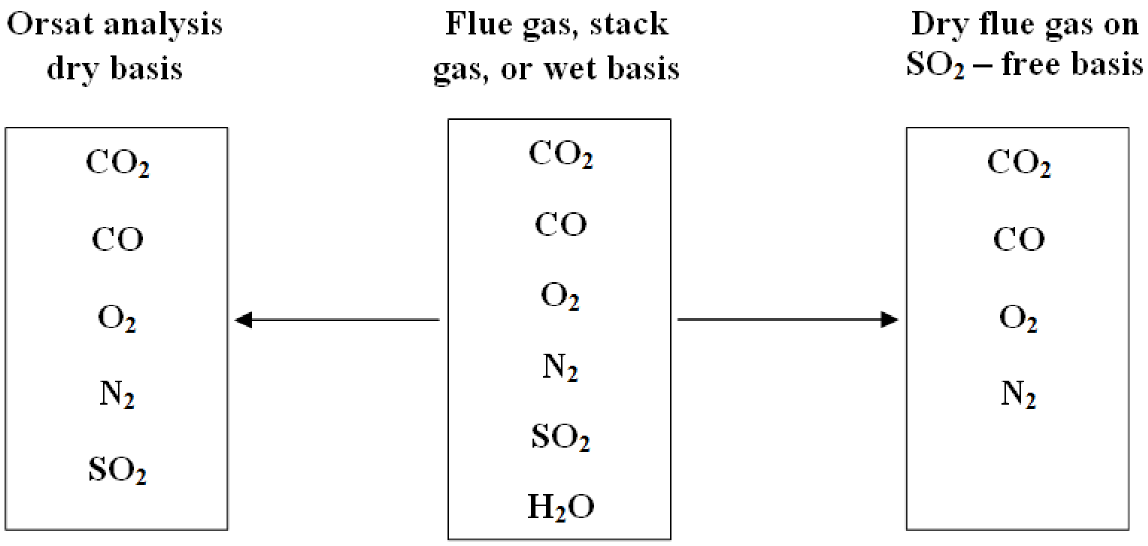
Material Balances Involving Combustion

Combustion is the reaction of a substance with oxygen with the associated release of energy and generation of product gases such as H_2O, CO_2, CO, and SO_2. Typical examples of combustion are the combustion of coal, heating oil, and natural gas used to generate electricity in utility power stations, and engines that operate using the combustion of gasoline or diesel fuel. Most combustion processes use air as the source of oxygen.

Combustion requires special attention because of some of the terminology involved. You should become familiar with these special terms:

a. **Flue or stack gas:** all the gases resulting from a combustion process including the water vapor, sometimes known as **a wet basis**.

b. **Orsat analysis or dry basis**: all the gases resulting from a combustion process not including the water vapor. (Orsat analysis refers to a type of gas analysis apparatus in which the volumes of the respective gases are measured over and in equilibrium with water; hence each component is saturated with water vapor. The net result of the analysis is to eliminate water as a component that is measured.) Look at Figure below. To convert from one analysis to another, you have to adjust the percentages of the components to the desired basis.



c. **Complete combustion**: the complete reaction of the hydrocarbon fuel producing CO_2, SO_2, and H_2O.

d. **Partial combustion**: the combustion of the fuel producing at least some CO. Because CO itself can react with oxygen, the production of CO in a combustion process does not produce as much energy as it would if only CO_2 were produced.

e. Fuels: The fuel used in power plant combustion furnaces may be solids, liquids or gases.

1. **Solid fuels:** Principally coal is the most important classical and natural fuel. It consists of **(a)** element carbon **(b)** complex of unknown structure consists of C, H, O, N and S **(c)** non-combustible matter that forms the ash.

2. **Liquid fuels:** Principally hydrocarbons obtained from distillation of crude oil such as gasoline, kerosene, diesel oil and fuel oil. However, there is growing interest to use alcohols obtained by fermentation of grains as liquid fuel.

3. **Gas fuels:** Principally natural gas is an important gaseous fuel. It consists of 80-90% CH_4, the reminder being ethane, propane and small quantities of other gases. However, light hydrocarbons obtained from petroleum or coal treatment such as producer gas, blast-furnace gas and refinery gas are examples of synthetic gaseous fuels. Acetylene and hydrogen can be also used as fuels but their production are relatively expensive.

f. Heating or Calorific values of fuels: is defined as the total heat produced when a unit mass of fuel is completely burnt with pure oxygen. When water is present in the flue gases, the heating value is said " higher heating value (HHV)". If the water is present in the liquid form; and it is said " lower heating value (LHV)". If the water is present in the vapour form ; i.e. a quantity of heat equal to the latent heat of vaporization of water. Higher heating values for common fuels are given in the table below. It is clear that H_2 is the best fuel but it is not present naturally in any appreciable quantities and its production cost is high which makes it less economical mean other fuels in the table.

Typical heating values of common fuels

	Higher heating value	
Fuel	**kJ/g**	**Btu/Ib_m**
Wood	17	7700
Soft coal	23	10000
Hard coal	35	15000
Fuel oil, gasoline	44	19000
Natural gas	54	23000
Hydrogen	143	61000

g. Air: is the source of oxygen in most combustion processes for obvious economic reasons. Air has the following composition:

N_2	78.03 mol %
O_2	20.99 mol %
Ar	0.94 mol%
H_2, He, Ne, Kr, Xe	0.01 mol%

Average molecular weight = 29.0 kg/kgmol
The volume of 1 Ibmole under 77.7 ^{o}F
& 1 atm is equal to 392 ft^3

However, combustion calculations are usually carried out with composition of 79 mol% of N_2 and 21 mol% of O_2 to simplify such calculations.

f. Theoretical air (or theoretical oxygen): the minimum amount of air (or oxygen) required to be brought into the process for complete combustion according to the stoichiometric requirement. Sometimes this quantity is called the required air (or oxygen).

g. Excess air (or excess oxygen): is the amount of air (or oxygen) in excess of that required for complete combustion as defined in (c). The calculated amount of excess air does not depend on how much material is actually burned but what is possible to be burned. Even if only partial combustion takes place, as, for example, **C** burning to both **CO** and **CO_2**, the excess air (or oxygen) is computed as if the process of combustion went to completion and produced only **CO_2**.

$$\%\ \text{excess air} = \frac{\text{excess air}}{\text{theoretical air}} \times 100 = \frac{\text{excess } O_2/0.21}{\text{theoretical } O_2/0.21} \times 100$$

$$\%\ \text{excess air} = \frac{\text{excess } O_2}{\text{theoretical } O_2} \times 100 = \frac{\text{entering } O_2 - \text{theoretical } O_2}{\text{theoretical } O_2} \times 100$$

It is important to note that heat losses through the flue gases increases with increasing % excess air, hence it is better to choose the optimum value of % excess air depending on type of the fuel as given in the table below.

Excess air for fuels

Fuels	**% Excess air**
Solids	25 – 60
Liquids	15 – 35
Gases	10 - 20

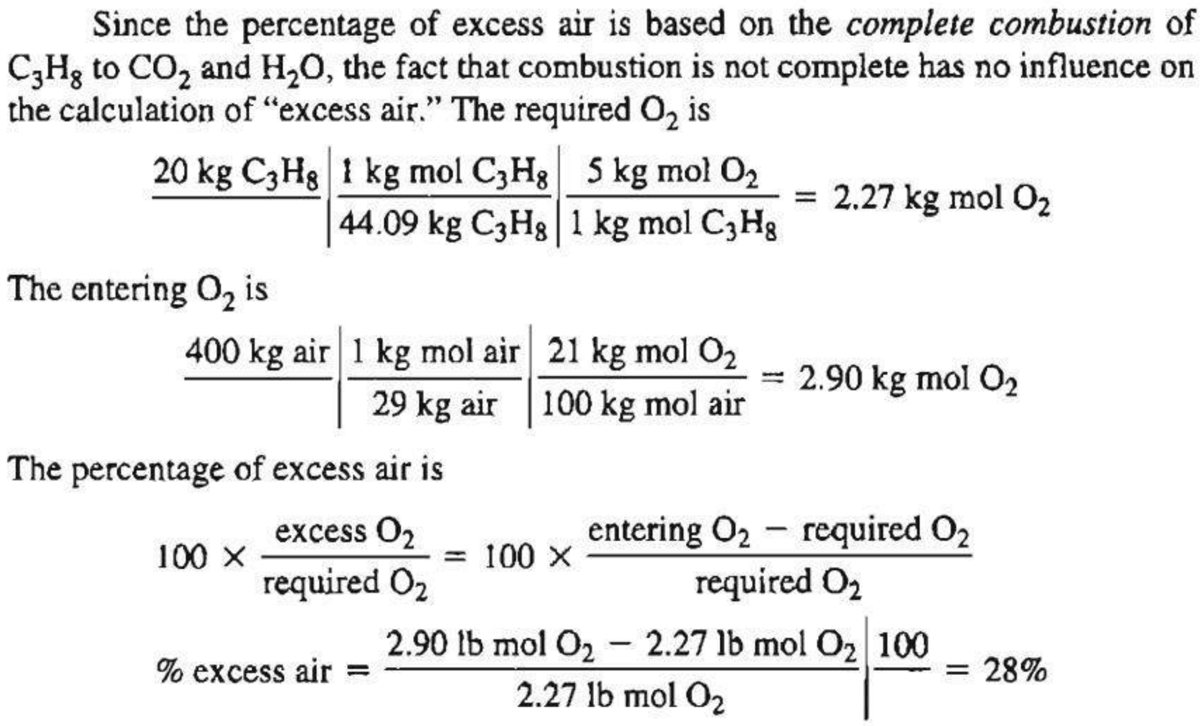
<u>Example 10.7:</u> Excess Air

Suppose that in a test 20 kg of propane (C_3H_8) is burned with 400 kg of air to produce 44 kg CO_2 and 12 kg of CO. What was the percentage excess air?

Solution:

$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$

Basis: 20 kg of C_3H_8



Since the percentage of excess air is based on the *complete combustion* of C_3H_8 to CO_2 and H_2O, the fact that combustion is not complete has no influence on the calculation of "excess air." The required O_2 is

$$\frac{20\text{ kg }C_3H_8}{}\left|\frac{1\text{ kg mol }C_3H_8}{44.09\text{ kg }C_3H_8}\right|\frac{5\text{ kg mol }O_2}{1\text{ kg mol }C_3H_8} = 2.27\text{ kg mol }O_2$$

The entering O_2 is

$$\frac{400\text{ kg air}}{}\left|\frac{1\text{ kg mol air}}{29\text{ kg air}}\right|\frac{21\text{ kg mol }O_2}{100\text{ kg mol air}} = 2.90\text{ kg mol }O_2$$

The percentage of excess air is

$$100 \times \frac{\text{excess }O_2}{\text{required }O_2} = 100 \times \frac{\text{entering }O_2 - \text{required }O_2}{\text{required }O_2}$$

$$\%\text{ excess air} = \frac{2.90\text{ lb mol }O_2 - 2.27\text{ lb mol }O_2}{2.27\text{ lb mol }O_2}\left|\frac{100}{}\right. = 28\%$$

<u>Example 10.8:</u> A fuel Cell to Generate Electricity from Methane

A fuel cell is an open system into which fuel and air are fed, and out of which comes electricity and waste products. Figure E10.8 is a sketch of a fuel cell in which a continuous flow of methane (CH_4) and air (O_2 plus N_2) produce electricity plus CO_2 and H_2O. Special membranes and catalysts are needed to promote the reaction of CH_4. Based on the data given in Figure E10.8, you are asked to calculate the composition of the products in **P**.

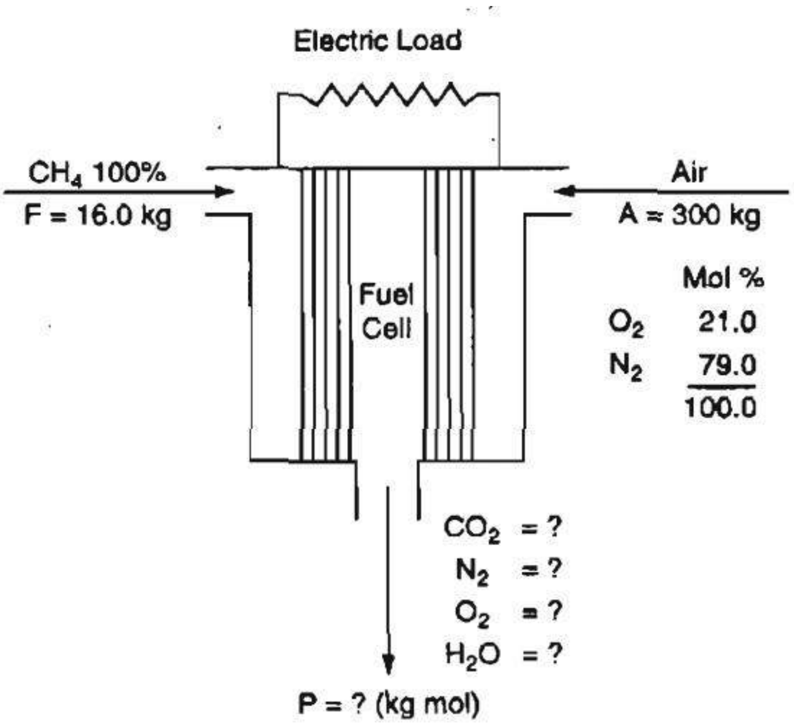


Figure E10.8

Solution:

This is a steady-state process with reaction. We have a complete reaction because no CH_4 in product.

Basis: 16 kg of CH_4 entering = 1 kgmol CH_4

$$\frac{300\ \text{kg A}}{}\left|\frac{1\ \text{kg mol A}}{29.0\ \text{kg A}}\right. = 10.35\ \text{kg mol A in}$$

$$\frac{16.0\ \text{kg CH}_4}{}\left|\frac{1\ \text{kg mol CH}_4}{16.0\ \text{kg CH}_4}\right. = 1.00\ \text{kg mol CH}_4\ \text{in}$$

$$\frac{10.35\ \text{kg mol A}}{}\left|\frac{0.21\ \text{kg mol O}_2}{1\ \text{kg mol A}}\right. = 2.17\ \text{kg mol O}_2\ \text{in}$$

$$\frac{10.35\ \text{kg mol A}}{}\left|\frac{0.79\ \text{kg mol N}_2}{1\ \text{kg mol A}}\right. = 8.18\ \text{kg mol N}_2\ \text{in}$$

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

1. Element material balances: (4 independent)

C, H, O, N

	Out		In
C:	$n^P_{CO_2}(1)$	=	1(1)
H:	$n^P_{H_2O}(2)$	=	1(4)
O:	$n^P_{CO_2}(2) + n^P_{O_2}(2) + n^P_{H_2O}(1)$	=	2.17(2)
2N:	$n^P_{N_2}$	=	8.18

2. Species material balances:

$$n_i^{out} = n_i^{in} + \xi \nu_i$$

Compound	Out		In		$\nu_i\xi$		g mol
CH_4:	$n^P_{CH_4}$	=	1.0	−	1 × 1	=	0
O_2:	$n^P_{O_2}$	=	2.17	−	2 × 1	=	0.17
N_2:	$n^P_{N_2}$	=	8.18	−	0 × 1	=	8.18
CO_2:	$n^P_{CO_2}$	=	0	+	1 × 1	=	1.0
H_2O:	$n^P_{H_2O}$	=	0	+	2 × 1	=	2.0

P = 0.17 + 8.18 + 1.0 + 2.0 = 11.35 gmol

$y_{O_2} = 1.5\%$, $y_{N_2} = 72.1\%$, $y_{CO_2} = 8.8\%$, and $y_{H_2O} = 17.6\%$

Example 10.9: Combustion of Coal

A local utility burns coal having the following composition on a dry basis. (Note that the coal analysis below is a convenient one for our calculations, but is not necessarily the only type of analysis that is reported for coal. Some analyses contain much less information about each element.)

Component	Percent
C	83.05
H	4.45
O	3.36
N	1.08
S	0.70
Ash	7.36
Total	100.0

The average Orsat analysis of the gas from the stack during a 24-hour test was:

Component	Percent
$CO_2 + SO_2$	15.4
CO	0.0
O_2	4.0
N_2	80.6
Total	100.0

Moisture in the fuel was 3.90% and the air on the average contained 0.0048 Ib H_2O/Ib dry air. The refuse showed 14.0% unburned coal, with the remainder being ash. You asked to check the consistency of the data before they are stored in a database. Is the consistency satisfactory? What was the average excess air used?

Solution:

This is an open, steady state process with reaction. The system is the furnace.

All the information given in the problem statement has been placed on figure E10.9. Because the gas analysis is on dry basis, we added a flowstream ***W*** for the exit water to the process diagram.

The composition of ***F*** and ***R*** are given in mass, and those of ***P*** and ***A*** moles.

Basis of ***F*** = 100 Ib as convenient

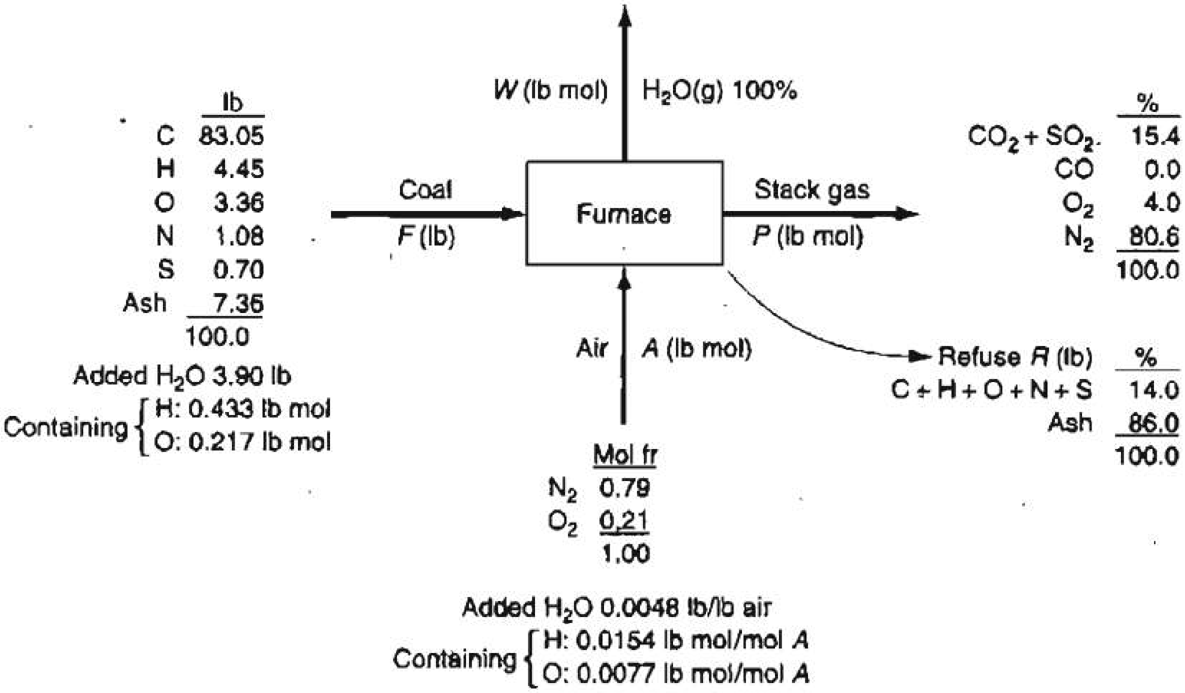


Figure E10.9

You must first calculate some extra information besides the compositions given in the diagram (the information has already been added to Figure E10.9 for convenience).

H_2O in coal:

$$\frac{3.90 \text{ lb } H_2O}{} \left| \frac{1 \text{ lb mol } H_2O}{18 \text{ lb } H_2O} \right| \frac{2 \text{ lb mol H}}{1 \text{ lb mol } H_2O} = 0.433 \text{ lb mol H}$$

(with 0.217 lb mol O)

H_2O in air:

$$\frac{0.0048 \text{ lb } H_2O}{\text{lb air}} \left| \frac{29 \text{ lb air}}{1 \text{ lb mol air}} \right| \frac{1 \text{ lb mol } H_2O}{18 \text{ lb } H_2O} = 0.0077 \frac{\text{lb mol } H_2O}{\text{lb mol air}}$$

(with 0.0154 lb mol H/lb mol A)
(with 0.0077 lb mol O/lb mol A)

You might neglect the C, H, O, N, and S in the refuse, but we will include the amount to show what calculations would be necessary if the amounts of the elements were significant. To do so, we must make a preliminary mass balance for the ash

$$\text{ash balance (lb)}: 7.36 = 0.86(R)$$

$$R = 8.56 \text{ lb}$$

The unburned coal in the refuse is

$$8.56(0.14) = 1.20 \text{ lb}$$

If we assume that the combustibles in the refuse occur in the same proportions as they do in the coal (which may not be true), the quantities of the combustibles in *R* on an ash-free basis are:

Component	mass %	lb	lb mol
C	89.65	1.076	0.0897
H	4.80	0.058	0.0537
O	3.63	0.0436	0.0027
N	1.17	0.014	0.0010
S	0.76	0.009	0.0003
	100.00	1.20	0.1474

The element balances in Ibmoles are:

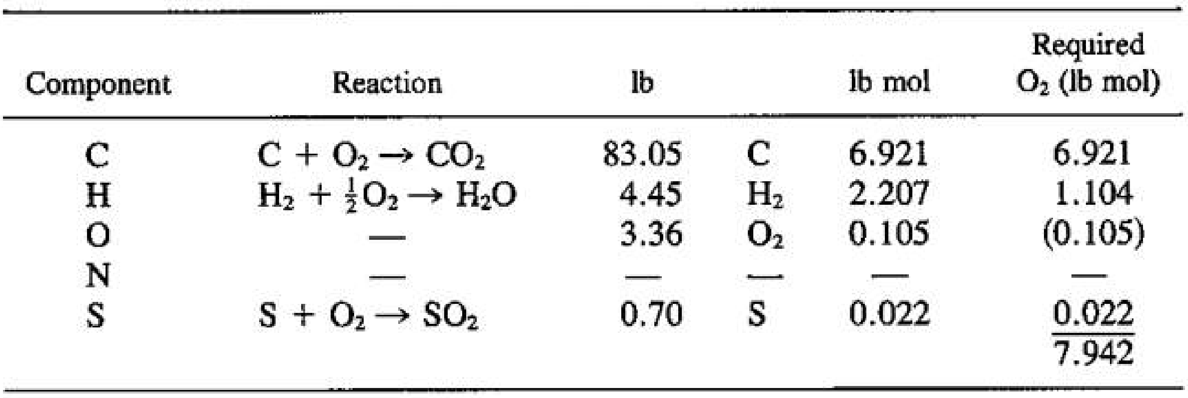
	In		Out		
	F	A	W	P	R
C + S:	$\frac{83.05}{12.0} + \frac{0.70}{32.0}$ +	0	= 0 +	$P(0.154)$ +	0.0897+0.0003
H:	$\frac{4.45}{1.008}$ + 0.433 +	0.0154 *A*	= 2*W* +	0 +	0.0537
O:	$\frac{3.36}{16.0}$ + 0.217 +	0.21*A*(2)+0.007*A*	= *W* +	2*P*(0.154+0.040) +	0.0027
N:	$\frac{1.08}{14.0}$ +	2(0.79A)	= 0 +	2*P*(0.806) +	2(0.001)

Solve the above equations to find:

P = 44.5 Ibmole , A = 45.35 Ibmole and W = 2.747 Ibmole

$$\% \text{ excess air} = \frac{\text{entering } O_2 - \text{theoretical } O_2}{\text{theoretical } O_2} \times 100$$

The required air is:



Component	Reaction	lb		lb mol	Required O_2 (lb mol)
C	$C + O_2 \rightarrow CO_2$	83.05	C	6.921	6.921
H	$H_2 + \frac{1}{2}O_2 \rightarrow H_2O$	4.45	H_2	2.207	1.104
O	—	3.36	O_2	0.105	(0.105)
N	—	—	—	—	—
S	$S + O_2 \rightarrow SO_2$	0.70	S	0.022	0.022
					7.942

The entering oxygen in the air is (45.35)(0.21) = 9.524 Ibmole

$$\% \text{ excess air} = \frac{9.524 - 7.942}{7.942} \times 100 = 19.9\%$$

H.W : 10.1, 10.4, 10.13, 10.16,10.18.

Chapter 11

Material Balance Problems Involving Multiple Units

<u>Example 11.2</u> : Multiple Units in Which No reaction Occurs :

Acetone is used in the manufacture of many chemicals and also as a solvent. In its later role, many restrictions are placed on the release of acetone vapor to the environment. You are asked to design an acetone recovery system having the flowsheet illustrated in Figure below. All the concentrations shown in Figure of both gases and liquids are specified in weight percent to make the calculations simpler. Calculate A, F, W, B and D per hour. G = 1400 kg/hr.

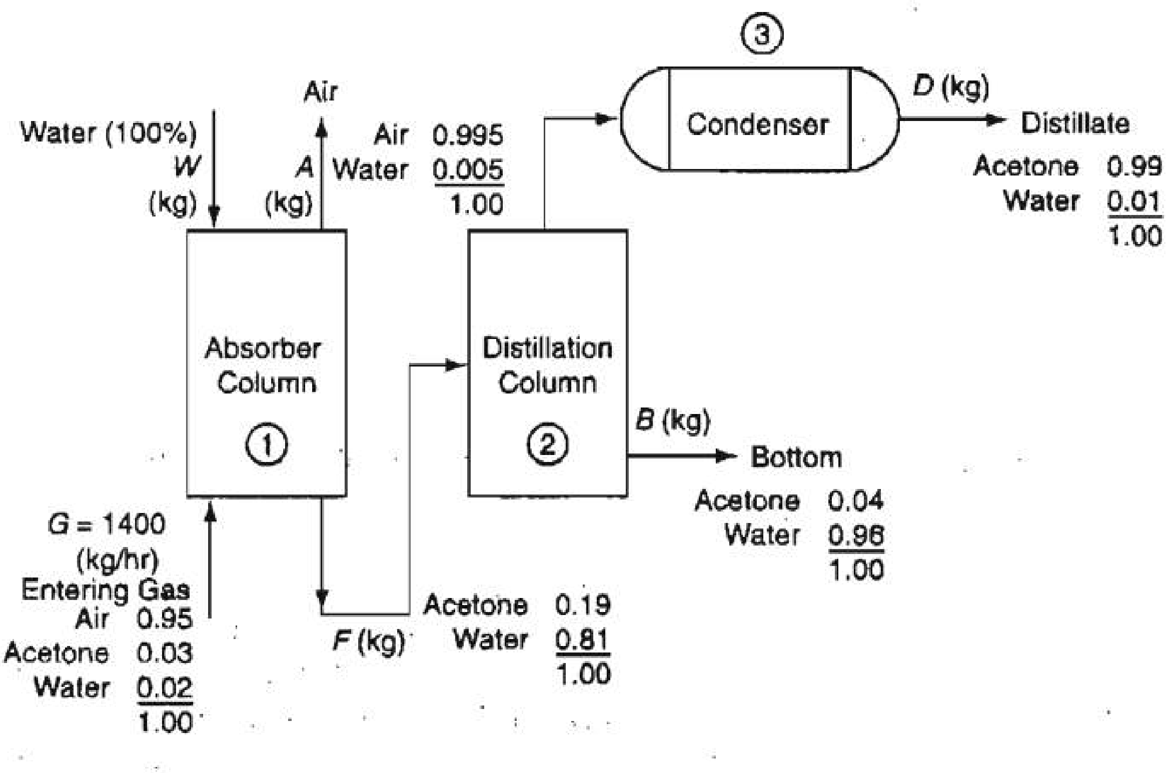


Figure E11.2

Solution:

Basis: 1 hr $\Longrightarrow$ G = 1400 kg

Material balance on absorption column:

a. Air balance (Tie component)
(0.95) (G) = (0.995) (A)
(0.95) (1400) = (0.995) (A) $\Longrightarrow$ **A = (1330/0.995) = 1336.7 kg**

b. Acetone balance
(0.03) (G) = (0.19) (F)
(0.03) (1400) = (0.19) (F) $\Longrightarrow$ **F = (42/0.19) = 221.05 kg**

c. Water balance
(0.02) (G) + (1.0) (W) = (0.81) (F)
(0.02) (1400) + (1.0) (W) = (0.81) (221.05) + (0.005) (A)
W = 157.7 kg

Checking: T.M.B
Input = G + W = 1400 + 157.7 = 1557.7 kg
Output = A + F = 1336.7 + 221.05 = 1557.7 kg

Material balance on distillation column:

a. Overall material balance:
F = D + B $\Longrightarrow$ D + B = 221.05 ………….. (1)

b. Acetone material balance:
(0.19) (F) = (0.99) (D) + (0.04) (B)
(0.19) (221.05) = (0.99) (D) + (0.04) (B)
51.9995 = (0.99) (D) + (0.04) (B) …………………….(2)

Solve Eq. (1) and Eq. (2) to get:
D = 34.91 kg
B = 186.1 kg

Checking: T.M.B
Input = F = 221.05 kg
Output = D + B = 186.1 + 34.91 = 221.01 kg

Example 11.4:

A simplified flowsheet for the manufacture of sugar is shown in Fig. E 11.4. Sugarcane is fed to a mill where a syrup is squeezed out, and the resulting "bagasse" contains 80% pulp. The syrup (E) containing finely divided pieces of pulp is fed to a screen which removes all the pulp and produces a clear syrup (H) containing 15% sugar and 85% water. The evaporator makes a "heavy" syrup and the crystallizer produces 1000 lb/hr of sugar crystals.

(a) Find the water removed in the evaporator, lb/hr.

(b) Find the composition of the waste stream G.
(c) Find the rate of feed of cane to the unit, lb/hr.
(d) Of the sugar fed in the cane, what percentage is lost with the bagasse?

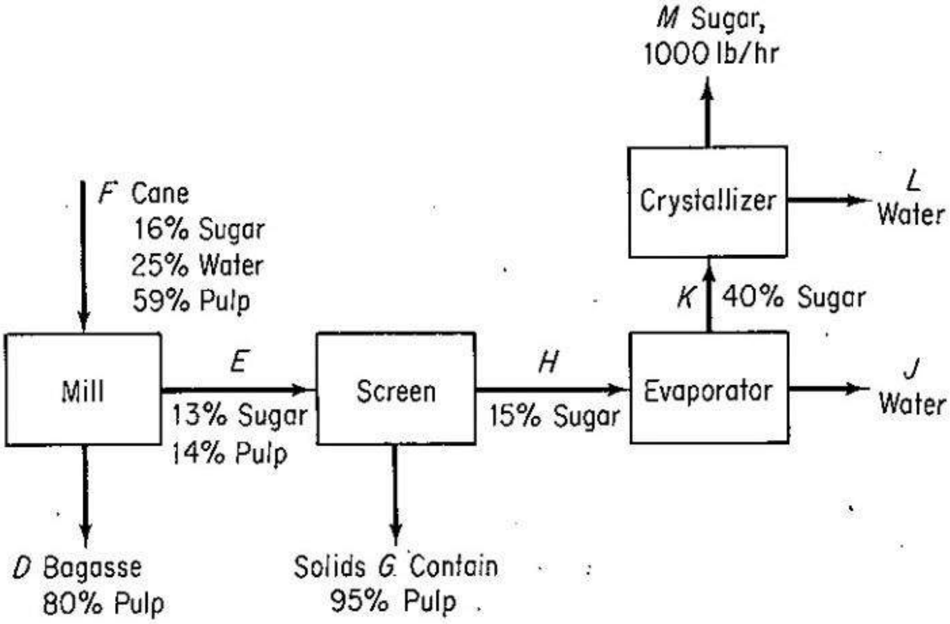


Figure E 11.4

Solution:

Basis: F =1000 Ib

1. **Material balance on Mill:**

   a. Pulp balance:

   (0.59) (F) = (0.14) (E) + (0.8) (D)
   (0.59) (1000) = (0.14) (E) + (0.8) (D)
   590 = 0.14 E + 0.8 D ……………………………(1)

   b. (Sugar + water) balance:

   (0.41) (F) = (0.86) (E) + (0.2) (D)
   (0.41) (1000) = (0.86) (E) + (0.2) (D)
   410 = 0.86 E + 0.2 D ……………………………(2)

Sub. Eq.(1) in Eq.(2):

410 = 0.2 ((590-0.14 E)/0.8) + 0.86 E
410 = 147.5 – 0.035 E + 0.86 E
0.825 E =262.5
E = 318.2 Ib

Sub. (E) in Eq.(1):
D = ((590 - 0.14 E)/0.8) = ((590 - 0.14 * 318.2)/0.8)= 681.8 Ib

Checking: T.M.B
Input = F = 1000 Ib
Output = E + D = 318.2 + 681.8 = 1000 Ib

c. Sugar balance:
(0.16) (F) = (0.13) (E) + (x) (D), Where: x= mass fraction of sugar in D
(0.16) (1000) = (0.13) (318.2) + (x) (681.8)
x = 0.174

d. Water balance:
(0.25) (F) = (0.73) (E) + (y) (D), Where: y= mass fraction of water in D
(0.25) (1000) = (0.73) (318.2) + (y) (681.8)
y = 0.026

Checking:
x + y = 0.174 + 0.026 = 0.2

2. Material balance on Screen:

a. Pulp balance:
(0.14) (E) = (0.95) (G)
(0.14) (318.2) = (0.95) (G)
G = 46.9 Ib

b. (Sugar + water) balance:
(0.86) (E) = (0.05) (G) + (1.0) (H)
(0.86) (318.2) = (0.05) (46.9) + (1.0) (H)
H = 271.3 Ib

Checking: T.M.B
Input = E = 318.2 Ib
Output = G + H = 46.9 + 271.3 = 318.2 Ib

c. Sugar balance:
(0.13) (E) = (0.15) (H) + (x) (G), Where: y= mass fraction of sugar in G
(0.13) (318.2) = (0.15) (271.3) + (x) (46.9)
x = 0.014

d. Water balance:
(0.73) (E) = (0.85) (H) + (y) (G), Where: y= mass fraction of water in G
(0.73) (318.2) = (0.85) (271.3) + (y) (46.9)
y = 0.036

Checking:

x + y = 0.014 + 0.036 = 0.05

3. **Material balance on Evaporator:**
   a. **Sugar balance:**
      (0.15) (H) = (0.4) (K)
      (0.15) (271.3) = (0.4) (K)
      K = 101.7 Ib

   b. **Water balance:**
      (0.85) (H) = (1.0) (V) + (0.6) (K)
      (0.85) (271.3) = (1.0) (V) + (0.6) (101.7)
      V = 169.6 Ib

Checking: T.M.B

Input = H = 271.3 Ib

Output = V + K = 169.6 + 101.7 = 271.3 Ib

4. **Material balance on Crystallizer:**
   a. **Sugar balance:**
      (0.4) (K) = (1.0) (M)
      (0.4) (101.7) = (1.0) (M)
      M = 40.7 Ib

   b. **Water balance:**
      (0.6) (K) = (1.0) (L)
      (0.6) (101.7) = (1.0) (L)
      L = 61 Ib

Checking: T.M.B

Input = K = 101.7 Ib

Output = L + M = 61 + 40.7 = 101.7 Ib

Final checking: T.M.B

Input = F = 1000 Ib

Output = D + G + V + L + M = 681.8 + 46.9 + 169.9 + 61 + 40.7 = 1000 Ib

Change the basis to 1000 Ib of M:

F	D	E	G	H	V	K	L	M
1000	681.8	318.2	46.9	271.3	169.9	101.7	61	40.7
24570	16752	7818	1152	6666	4167	2499	1499	1000

<u>Example 11.3 </u>: Material balances for a process involving multiple units and reactions

In the face of the higher fuel costs and the uncertainty of the supply of a particular fuel, many companies operate two furnaces, one fired with natural gas and the other with fuel oil. In the RAMAD Corp., each has its own supply of oxygen. The furnace uses air while the oil furnace uses an oxidation stream that analyses: O_2, 20% ; N_2, 76%; and CO_2, 4%. The stack gases go up a common stack. See Figure E 11.3.

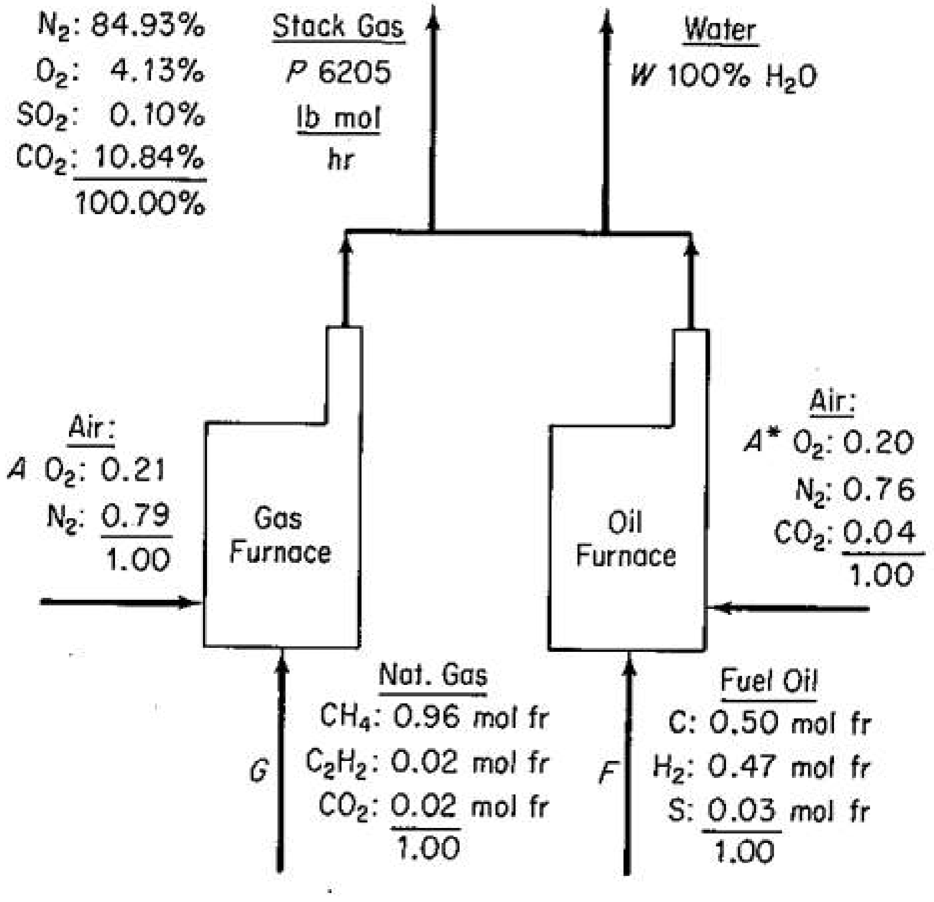
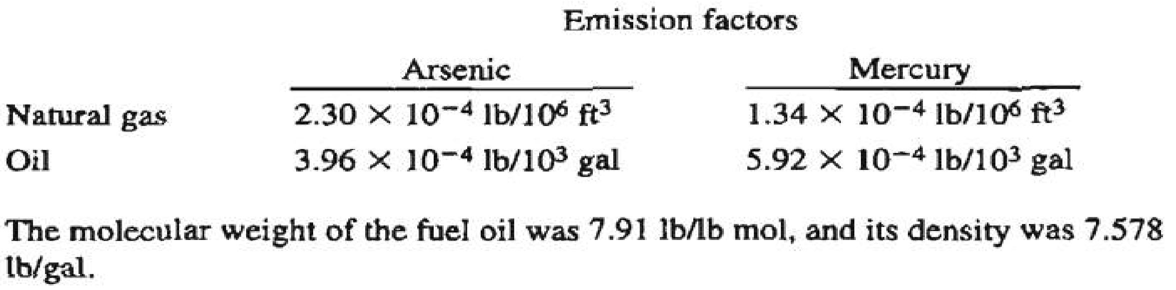


Figure E11.3

The reserve of the fuel oil was only 560 bbl. How many hours could the company operate before shutting down if no additional fuel was attainable? How many Ibmol/hr of natural gas were being consumed? The minimum heating. Also calculate the percent increase in toxic emission of arsenic and mercury per hour caused by the combustion of fuel oil rather than natural gas.



Emission factors

	Arsenic	Mercury
Natural gas	2.30×10^{-4} lb/10^6 ft^3	1.34×10^{-4} lb/10^6 ft^3
Oil	3.96×10^{-4} lb/10^3 gal	5.92×10^{-4} lb/10^3 gal

The molecular weight of the fuel oil was 7.91 lb/lb mol, and its density was 7.578 lb/gal.

Solution:

This is an open, steady-state process with reaction. Two subsystems exist. We want to calculate **F** and **G** in Ibmol/hr and then **F** in bbl/hr.

Basis: 1 hr so that P = 6205 Ibmol

The overall material balances for the elements in Ibmol are:

$$
\begin{array}{llcll}
 & \underline{\qquad\qquad In \qquad\qquad} & & \underline{\qquad\qquad Out \qquad\qquad} \\
2H: & G(1.94) + F(0.47) & = & W(1) \\
2N: & A(0.79) + A^{*}(0.76) & = & 6205(0.8493) \\
2O: & A(0.21) + A^{*}(0.20 + 0.04) & & 6205(0.0413 + 0.001 + 0.1084) \\
 & \qquad + G(0.02) & = & \qquad +W(\tfrac{1}{2}) \\
S: & F(0.03) & = & 6205(0.0010) \\
C: & G(0.96) + (2)(0.02) + 0.02 & & \\
 & \qquad + F(0.50) + 0.04A^{*} & = & 6205(0.1084)
\end{array}
$$

Solve the **S** balance for F, then solve for the other four balances simultaneously:

F = 207 Ibmol/hr G = 498 Ibmol/hr

Finally, the fuel oil consumption is

$$\frac{207\ \text{lb mol}}{\text{hr}}\left|\frac{7.91\ \text{lb}}{\text{lb mol}}\right|\frac{\text{gal}}{7.578\ \text{lb}}\left|\frac{\text{bbl}}{42\ \text{gal}}\right. = 5.14\ \text{bbl/hr}$$

If the fuel oil reserves were only 560 bbl, they could last at the most

$$\frac{560\ \text{bbl}}{5.14\dfrac{\text{bbl}}{\text{hr}}} = 109\ \text{hr}$$

The arsenic and the mercury produced are:

Fuel oil:

(5.14 bbl/hr)(42 gal/bbl) = 216 gal/hr

$$\text{Arsenic: } \frac{216\text{ gal}}{} \left| \frac{3.96 \times 10^{-4}\text{ lb}}{10^{3}\text{ gal}} \right. \approx 8.55 \times 10^{-5}\text{ lb}$$

$$\text{Mercury: } \frac{216\text{ gal}}{} \left| \frac{5.92 \times 10^{-4}\text{ lb}}{10^{3}\text{ gal}} \right. \approx 12.78 \times 10^{-5}\text{ lb}$$

Natural gas:

(498 lb mol/hr)(359 ft^3/lb mol) = 1.79 × 10^5 ft^3/hr

$$\text{Arsenic: } \frac{1.79 \times 10^{5}\text{ ft}^{3}}{} \left| \frac{2.30 \times 10^{-4}\text{ lb}}{10^{6}\text{ ft}^{3}} \right. = 4.11 \times 10^{-5}\text{ lb}$$

$$\text{Mercury: } \frac{1.79 \times 10^{-5}\text{ ft}^{3}}{} \left| \frac{1.34 \times 10^{-4}\text{ lb}}{10^{6}\text{ ft}^{3}} \right. = 2.40 \times 10^{-5}\text{ lb}$$

The increase in levels of arsenic and mercury are:

$$\text{Arsenic: } \frac{(8.55 - 4.11) \times 10^{-5}}{4.11 \times 10^{-5}}(100) = 108\%$$

$$\text{Mercury: } \frac{(12.78 - 2.40) \times 10^{-5}}{2.40 \times 10^{-5}}(100) \approx 433\%$$

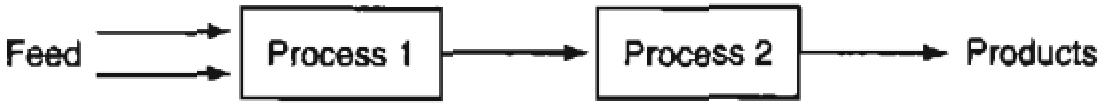
H.W : 11.1, 11.2, 11.7, 11.10, 11.15.

Chapter 12

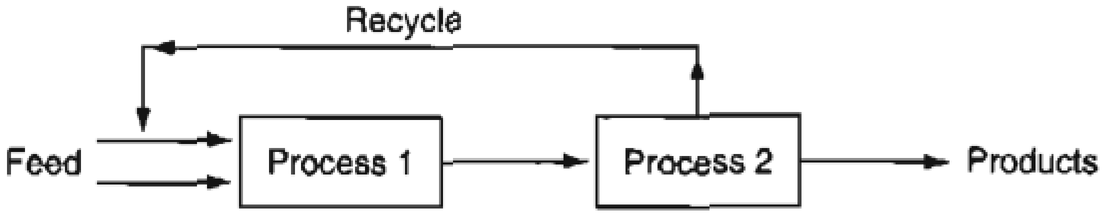
Recycle, Bypass, Purge, and the Industrial Application of Material Balances

Recycle, bypass and purge streams are commonly used in the design of chemical processes around the reaction units (reactors) as well as in unit operations such as drying, distillation and extraction units. Typical material balance calculations on a process involving such streams are given in this chapter.

(a) Single unit with serial flow



(b) Multiple units with serial flow

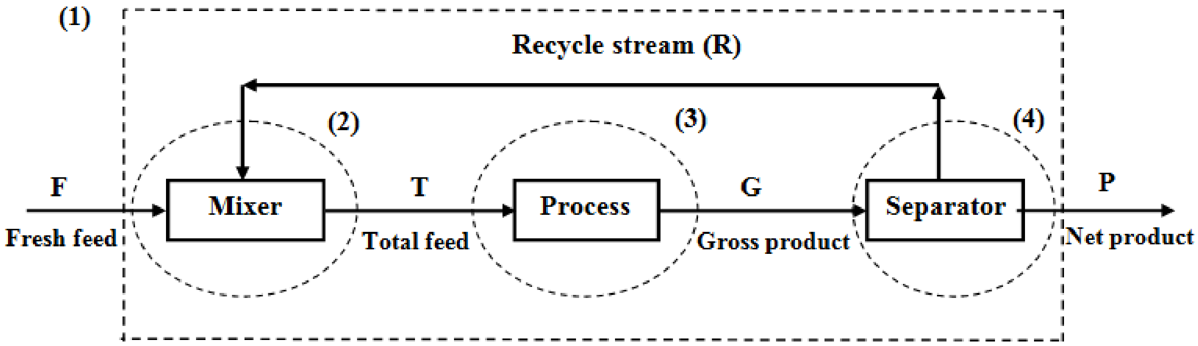


(C) Multiple units with recycle

Recycle stream:

It is part of the product stream (either similar or different composition) that is separated and returned to mix again with inlet stream (fresh feed) for economic considerations. The gross product (G) leaving the process is commonly separated by suitable separation technique such as distillation, filtration, extraction ……. etc, into the net product (P) and recycle stream

(R); whereas the inlet feed (T) input to the process is made up by mixing the fresh feed (F) and recycle stream (R) as shown in the following block diagram.



The recycle ratio, sometimes called reflux ratio, is widely used in recycle calculations. It is the ratio between the amount of recycle to that of the net product, i.e.$\left(\frac{R}{P}\right)$.

Material balance calculations can be made around:

1. The whole process.
2. The mixing unit.
3. The process only.
4. The separation unit.

The sequence of calculation steps depends on the data given in the problem.

* Note that the quantity of net product depends only on the quantity of the fresh feed. The quality of the recycle stream is charged once at the starting period of working the process and remains circulated inside the process with constant flow rate and composition under steady state conditions and it's value depends on the process conditions such as conversion and it is fixed according to economical considerations.

Here are some examples of the application of material recycling in the process industries:

1. **Increased reactant conversion**. Recycling the reactants back to the feed to a reactor can significantly increase the overall conversion of the reactants. For certain systems recycle allows the reactor to be operated at low conversion levels, yielding improved selectivity, with recycling of the unreacted reactants making it possible to attain a high overall degree of conversion.

2. **Continuous catalyst regeneration.** Catalysts are used to increase the rate of chemical reactions, but their effectiveness can diminish with use (catalyst deactivation). Processes that use catalysts that deactivate at a relatively fast rate may require the onsite regeneration and recycling of the catalyst. For example, in a fluidized catalytic cracking (FCC) process (Figure 12.4), the cracking catalyst deactivates almost immediately upon

contact with the gas oil feed at the reaction temperature because of the formation of coke on the surface of the catalyst. Therefore, the deactivated (spent) catalyst is transported to the catalyst regenerator where most of the coke is burned off the surface of the catalyst to restore the activity of the catalyst.

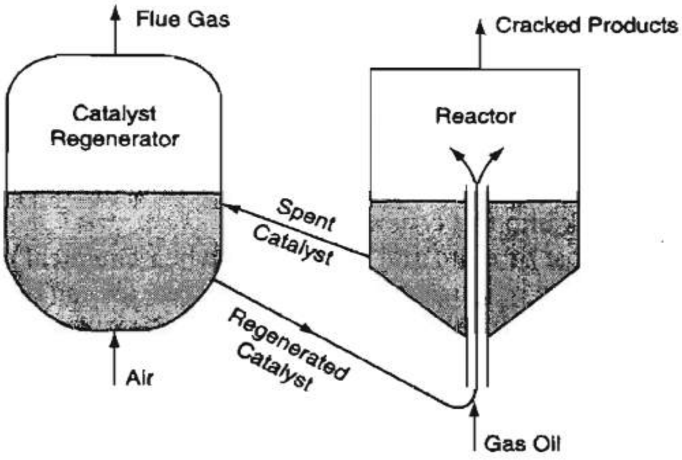


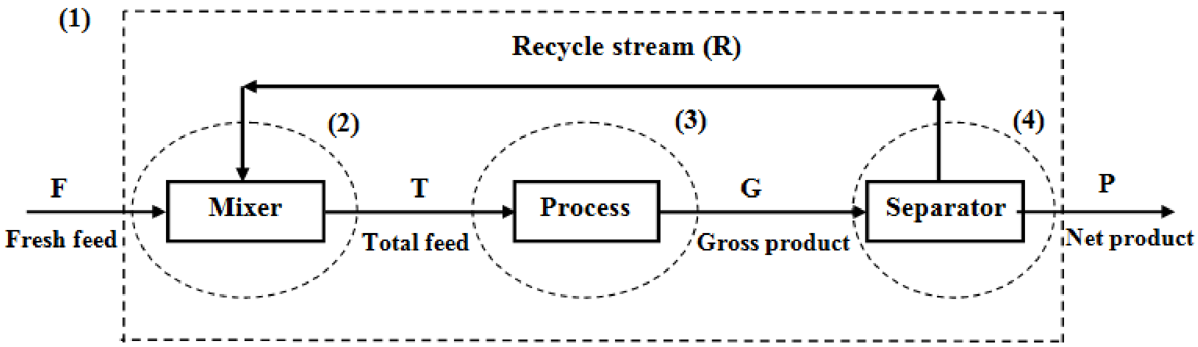
Figure 12.4 Diagram of a FCC process.

3. **Circulation of a working fluid**. A number of processes use the closed circulation of a working fluid for heating or refrigeration. Refrigeration systems, including home air conditioning systems, circulate a refrigerant gas by a compressor so that the gas absorbs heat from the room air and discharges heat to the outside atmosphere.

4. To maintain the required conditions to perform the process with higher efficiency such as recycling part of top product in rectification distillation from the top of the column.

5. To dilute the fresh feed such as recycling part of filtrate that leaves filtration unit to mix with fresh slurry since it is difficult to handle slurry with high solid concentration and the filter will operate more properly with recycle.

Recycle without chemical reaction



Material balance (1)

Fresh feed (F) = Net product (P)

Material balance (2)

Fresh feed (F) + Recycle (R) = Total feed (T)

Material balance (3)

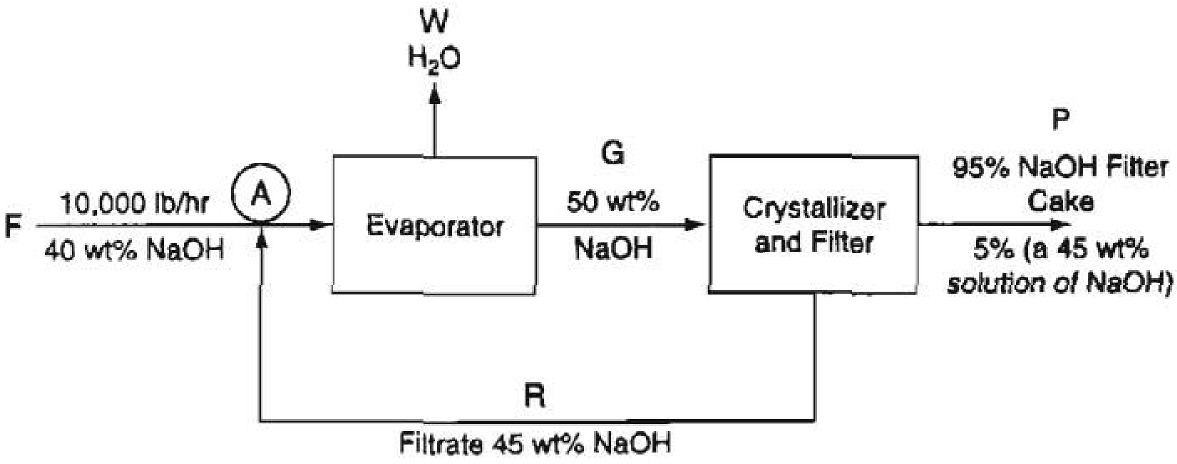
Total feed (T) = Gross product (G)

Material balance (4)

Gross product (G) = Recycle (R) + Net product (P)

Example 12.1: A continuous crystallizer involving a recycle stream

In block diagram below shows a process for the production of flake NaOH, which is used in households to clear plugged drain in the plumbing.



The fresh feed to the process is 10,000 lb/hr of a 40% aqueous NaOH solution. The fresh feed is combined with the recycled filtrate from the crystallizer, and fed to the evaporator where water is removed to produce a 50% NaOH solution, which in turn is fed to the crystallizer. The crystallizer produces a filter cake that is 95% NaOH crystals and 5% solution that itself consists of 45% NaOH. The filtrate contains 45% NaOH.

a. Calculate the flow rate of water removed by the evaporator, and the recycle rate for this process.

b. Assume that the same production rate of NaOH flakes occurs, but the filtrate is not recycled. What would be the total feed rate of 40% NaOH have to be then? Assume that the product solution from the evaporator still contains 50% NaOH.

Solution:

The process is open and steady state.

a. Basis: F = 10000 Ib fresh feed

Overall NaOH material balance:

(0.4) (10000) = [0.95 + (0.45) (0.05)] **P**

P = 4113 Ib

Overall H_2O material balance:

(0.6) (10000) = **W** + [(0.55) (0.05)] 4113

W = 5887 Ib

or use the overall material balance: **F** = **P** + **W**

10000 = 4113 + **W**

W = 5887 Ib

The total amount of NaOH exiting with **P** is :

[(0.95) + (0.45) (0.05)] (4113) = 4000 Ib

The amount of H_2O in **P** = [(0.55) (0.05)] 4113 = 113 Ib

As a check the total amount of H_2O in the output, 113 + 5887 = 6000 Ib

NaOH material balance on the crystallizer:

(0.5) **G** = 4000 + (0.45) **R** …………………(1)

H_2O material balance on the crystallizer:

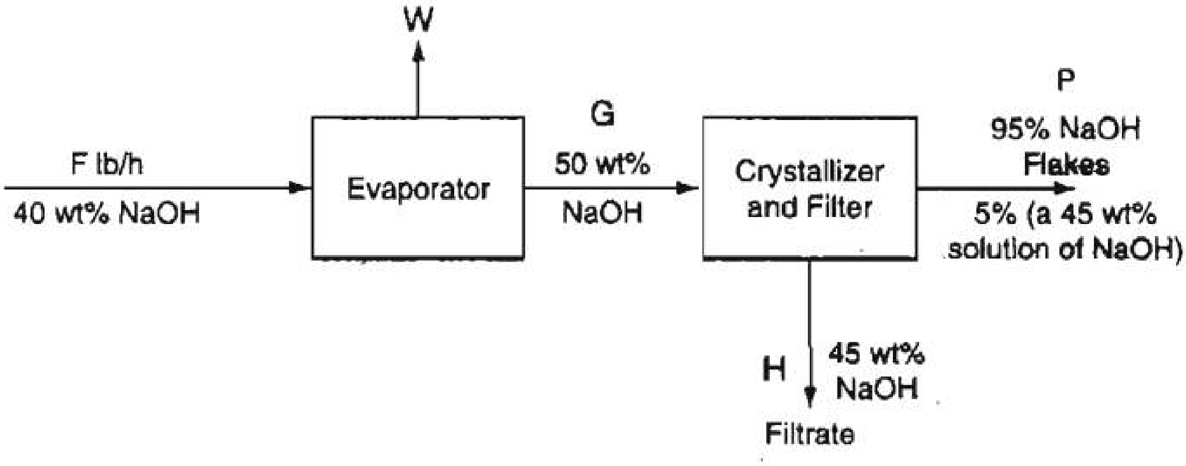
(0.5) **G** = 113 + (0.55) **R** …………………..(2)

or use total material balance: **G** = **R** + 4113

Solve Eq.(1) and Eq.(2) to get:

R = 38870 Ib

b. Now suppose recycle from crystallizer does not occur, but the production and composition of **P** remains the same.



The basis is now: **P** = 4113 Ib

NaOH material balance on the crystallizer:

(0.5) **G** = 0.45 **H** + [(0.95) + (0.05) (0.45)] (4113) …………………(3)

H_2O material balance on the crystallizer:

(0.5) **G** = 0.55 **H** + [(0.05) (0.55)] (4113) …………………..(4)

Solve Eq.(3) and Eq.(4) to get:

H = 38870 Ib

Overall material balance on the crystallizer:

G = **H** + **P**

G = 38870 + 4113 = 42983 Ib

Overall NaOH material balance:

(0.4) **F** = (0.45) **H** + [(0.05) (0.45)] **P**

(0.4) **F** = (0.45) 38870 + [(0.95) + (0.05) (0.45)] 4113

F = 53730 Ib

or NaOH material balance on the evaporator:

(0.4) **F** = (0.5) **G**

(0.4) **F** = (0.5) 42983

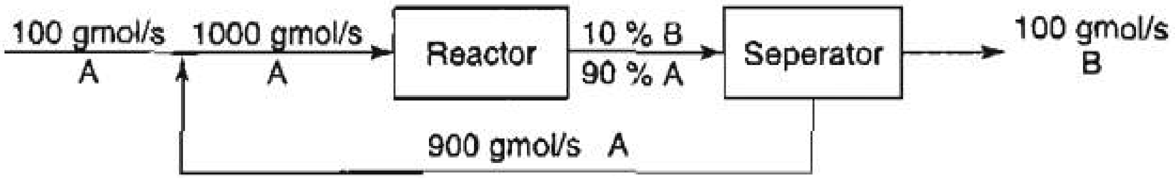
F = 53730 Ib

Not that without recycle, the feed rate must be 5.37 times larger than with recycle to produce the same amount of product.

Recycle with chemical reaction

Recycle of reactants that is used to increase the overall conversion in a rector. Figure below shows a simple example for the reaction.

$$A \rightarrow B$$



The extent of reaction for the overall process based on **B**:

$$\xi_{\text{overall}} = \frac{100 - 0}{1} = 100 \text{ moles reacting}$$

Material balance on reactor to calculate the output of the reactor:

A = 900 gmol

B = 100 gmol

The extent of reaction based on **B** for the reactor by itself as the system is:

$$\xi_{\text{reactor}} = \frac{100 - 0}{1} = 100 \text{ moles reacting}$$

**** In general, the extent of reaction is the same regardless of whether an overall material balance is used or a material balance for the reactor is used.***

There are two types of conversion when reactions occur:

1. Overall fraction conversion :

$$= \frac{mass\ (moles)\ of\ reactant\ in\ the\ fresh\ feed - mass\ (moles) of\ reactant\ in\ the\ output\ of\ the\ overall\ process}{mass\ (moles) of\ reactant\ in\ the\ fresh\ feed}$$

$$f_{\mathrm{OA}} = \frac{100-0}{100} = 100\%$$

2. Single – pass "once-through" fraction conversion:

$$= \frac{mass\ (moles)\ of\ reactant\ fed\ into\ the\ reactor - mass\ (moles) of\ reactant\ exiting\ the\ reactor}{mass\ (moles)\ of\ reactant\ fed\ into\ the\ reactor}$$

$$f_{\mathrm{SP}} = \frac{1000-900}{1000} = 10\%$$

* ***When the fresh feed consists of more than one reactant, the conversion can be expressed for a single component, usually the limiting reactant, or the most important (expensive) reactant.***

The overall conversion (f_{OA}) and the single-pass conversion (f_{SP}) can be expressed in terms of the extent of reaction as below:

$$\text{Overall conversion of species A} = f_{\mathrm{OA}} = \frac{-v_{\mathrm{A}}\xi}{n_{\mathrm{A}}^{\text{fresh feed}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

$$\text{Single-pass conversion} = f_{\mathrm{SP}} = \frac{-v_{\mathrm{A}}\xi}{n_{\mathrm{A}}^{\text{reactor feed}}} \quad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Material balance on mixing point:

$$n_{\mathrm{A}}^{\text{reactor feed}} = n_{\mathrm{A}}^{\text{fresh feed}} + n_{\mathrm{A}}^{\text{recycle}}$$

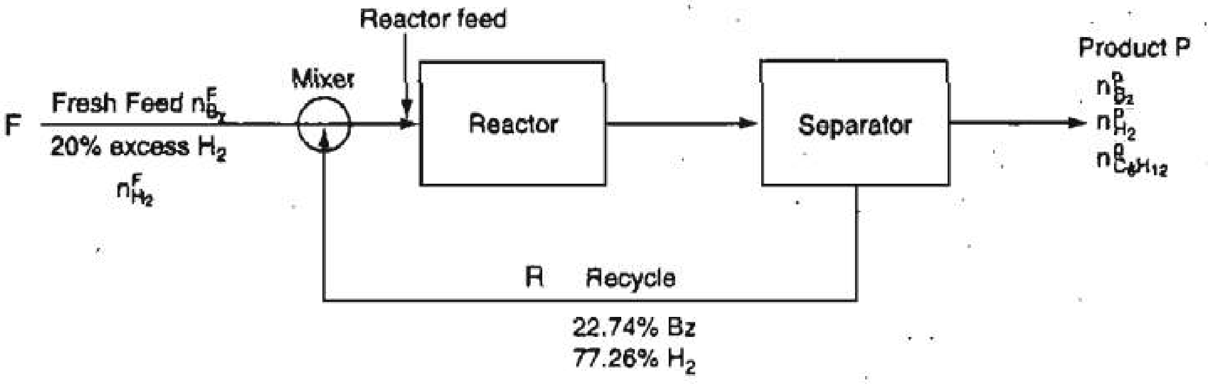
Divide Eq.(2) on the Eq.(1) to get:

$$\frac{f_{SP}}{f_{OA}} = \frac{n_A^{\text{fresh feed}}}{n_A^{\text{reactor feed}}} = \frac{n_A^{\text{fresh feed}}}{n_A^{\text{fresh feed}} + n_A^{\text{recycle}}}$$

Example 12.2: Cyclohexane (C_6H_{12}) can be made by the reaction of benzene (Bz) (C_6H_6) with hydrogen according to the following reaction:

$$C_6H_6 + 3H_2 \rightarrow C_6H_{12}$$

For the process shown below, determine the ratio of the recycle stream to the fresh feed stream if the overall conversion of benzene is 95%, and the single-pass conversion is 20%. Assume that 20% excess hydrogen is used in the fresh feed, and that the composition of the recycle stream is 22.74 mol % benzene and 77.26 mol % hydrogen.



Also calculate the environmental impact of the product gas by calculating an environmental index based on the following threshold limit values (TLV) for the respective components:

	TLV (ppm)
Benzene	0.5
Cyclohexane	300
Hydrogen	1000

Solution:

The process is open and steady state.

Basis: 100 mol fresh feed of benzene

The amount of H_2, which is in 20% excess (for complete reaction) is:

$$n^F_{H_2} = 100\,(3)(1+0.2) = 360\ \text{mol}$$

The total fresh feed = 100 + 360 = 460 mol

Overall conversion of species **Bz** $= f_{OBz} = \dfrac{-v_A \xi}{n_{Bz}^{\text{fresh feed}}}$

$\nu_{Bz} = -1$

$$0.95 = \frac{-(-1)\xi}{100}$$

ξ = 95 reacting moles

The unknown are: R, n_B^P , $n_{H_2}^P$ and $n_{C_6H_{12}}^P$

You can write three species balances for each of the three systems, the mixing point, the reactor and the separator plus overall material balance.

The species overall balances are :

$$n_i^{out} = n_i^{in} + \nu_i \xi_{overall}$$

$$\begin{aligned} &\text{Bz:} & n_{Bz}^P &= 100 + (-1)(95) &= 5 \text{ mol} \\ &H_2\text{:} & n_{H_2}^P &= 360 + (-3)(95) &= 75 \text{ mol} \\ &C_6H_{12} & n_{C_6H_{12}}^P &= 0 + (1)(95) &= \underline{95 \text{ mol}} \\ & & & & P = 175 \text{ mol} \end{aligned}$$

The recycle (R) can be calculated from the single-pass conversion:

Single-pass conversion $= f_{SP} = \dfrac{-v_A \xi}{n_{Bz}^{\text{reactor feed}}}$

$$0.2 = \frac{-(-1)\ 95}{100 + 0.2274\ R}$$

R = 1649 mol

Finally, the ratio of recycle to fresh feed is:

$$\frac{R}{F} = \frac{1649}{460} = 3.58$$

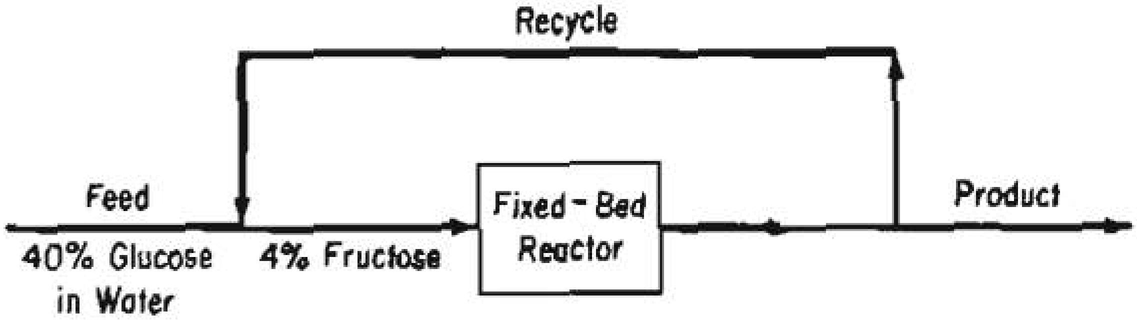
The higher the TLV, the more exposure that can be tolerated, hence an index should use the inverse of the TLV values appropriately weighed. You can use relative concentrations or mole fractions as weights.

$$\text{Environmental index} = \frac{5}{175}\left(\frac{1}{0.5}\right) + \frac{95}{175}\left(\frac{1}{300}\right) + \frac{75}{175}\left(\frac{1}{1000}\right) = 0.059$$

Note that the benzene contributes 96% of the index.

<u>Example 12.3</u>: Fructose is produced from glucose in a fixed-bed reactor (water is the solvent) From the figure below, what percent conversion of glucose results on one pass through the reactor when the ratio of the exit stream to the recycle stream in mass units is equal to 8.33? The reaction is:

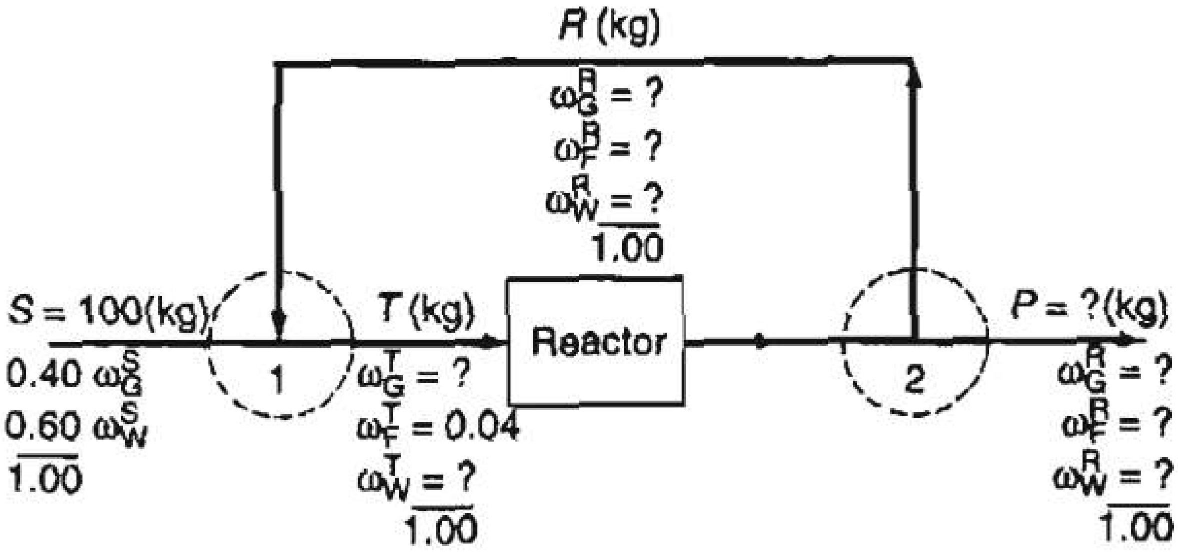
$$\underset{\text{Glucose}}{C_{12}H_{22}O_{11}} \rightarrow \underset{\text{Fructose}}{C_{12}H_{22}O_{11}}$$



Solution:

Note that the recycle stream and the product stream have the same composition.

Basis: 100 kg of feed (S)



Let **f** = fraction conversion for one pass through the reactor. The unknown are:

$R, P, T, \omega_G^R, \omega_F^R, \omega_W^R, \omega_G^T, \omega_W^T$, and f, for a total of 9.

The balances are $\Sigma\omega_i^R = 1$, $\Sigma\omega_i^T = 1$, $R = P/8.33$

Overall balances

Total: $P = S = 100$ kg (How simple!)

Consequently, $R = \dfrac{100}{8.33} = 12.0$ kg

Overall no water is generated or consumed, hence

Water: $100(0.60) = P\omega_W^R = 100\omega_W^R$

$\omega_W^R = 0.60$

No reaction occurs so that species balances can be used without involving th extent of reaction:

Total: $100 + 12 = T = 112$

Glucose: $100(0.40) + 12\omega_G^R = 112\omega_G^T$

Fructose: $0 + 12\omega_F^R = 112(0.04)$

$$\omega_F^R = 0.373$$

Also, because $\omega_F^R + \omega_G^R + \omega_W^R = 1,$

$$\omega_G^R = 1 - 0.373 - 0.600 = 0.027$$

$$\omega_G^T = 0.360$$

<u>Material balance on reactor and separator:</u>

Total M.B.: $T = P + R$

$T = 12 + 100 = 112$ kg

The fractional conversion of the single-pass through the reactor:

$$f_{sp} = \frac{mass\ of\ reactant\ fed\ into\ the\ reactor - mass\ of\ reactant\ exiting\ the\ reactor}{mass\ \ of\ reactant\ fed\ into\ the\ reactor}$$

$$f_{sp} = \frac{(\omega_G^T)\ T - (R + P)\ \omega_G^R}{(\omega_G^T)\ T}$$

$$f_{sp} = \frac{(0.36)(112) - (12 + 100)\ (0.027)}{(0.36)(112)}$$

$$f_{sp} = 0.93$$

<u>For checking:</u>

$$The\ extent\ of\ reaction\ = \frac{(\omega_G^R)\ (R + P) - (0.4)\ S}{-1}$$

$$The\ extent\ of\ reaction\ = \frac{(0.027)\ (112) - (0.4)\ 100}{-1}$$

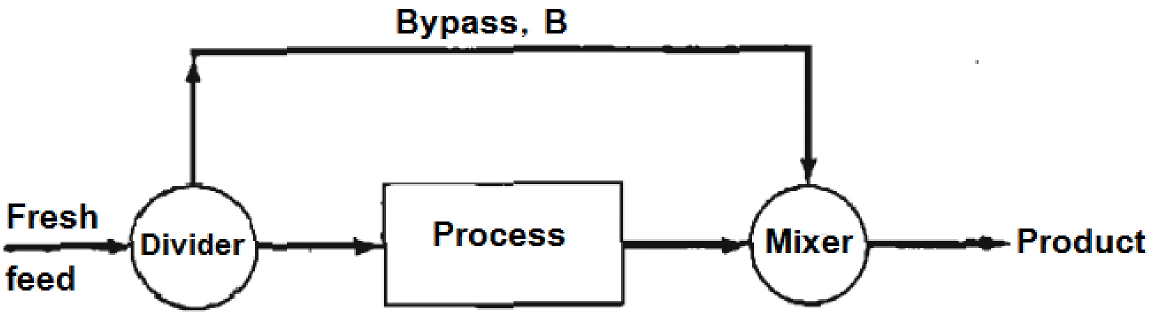
$$\xi = \frac{3.02 - 40}{-1} = 37$$

$$\text{Single-pass conversion} = f = \frac{-v_G\,\xi}{n_G^{\text{reactor feed}}}$$

$$f = \frac{-(-1)(37)}{40} = 0.93$$

Bypass and Purge

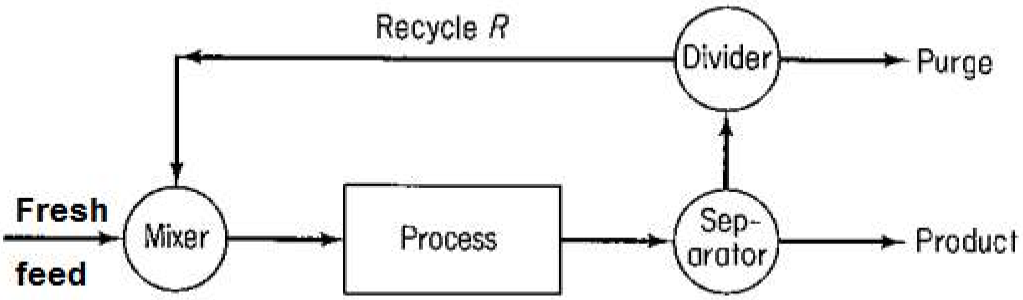
a. **Bypass stream:** It is a fraction of the fresh feed that skips one or more stages of the process and goes directly to downstream stage as shown in the block diagram below. This arrangement is used when it is desired to control the composition of the final exit stream (product) at desired value.



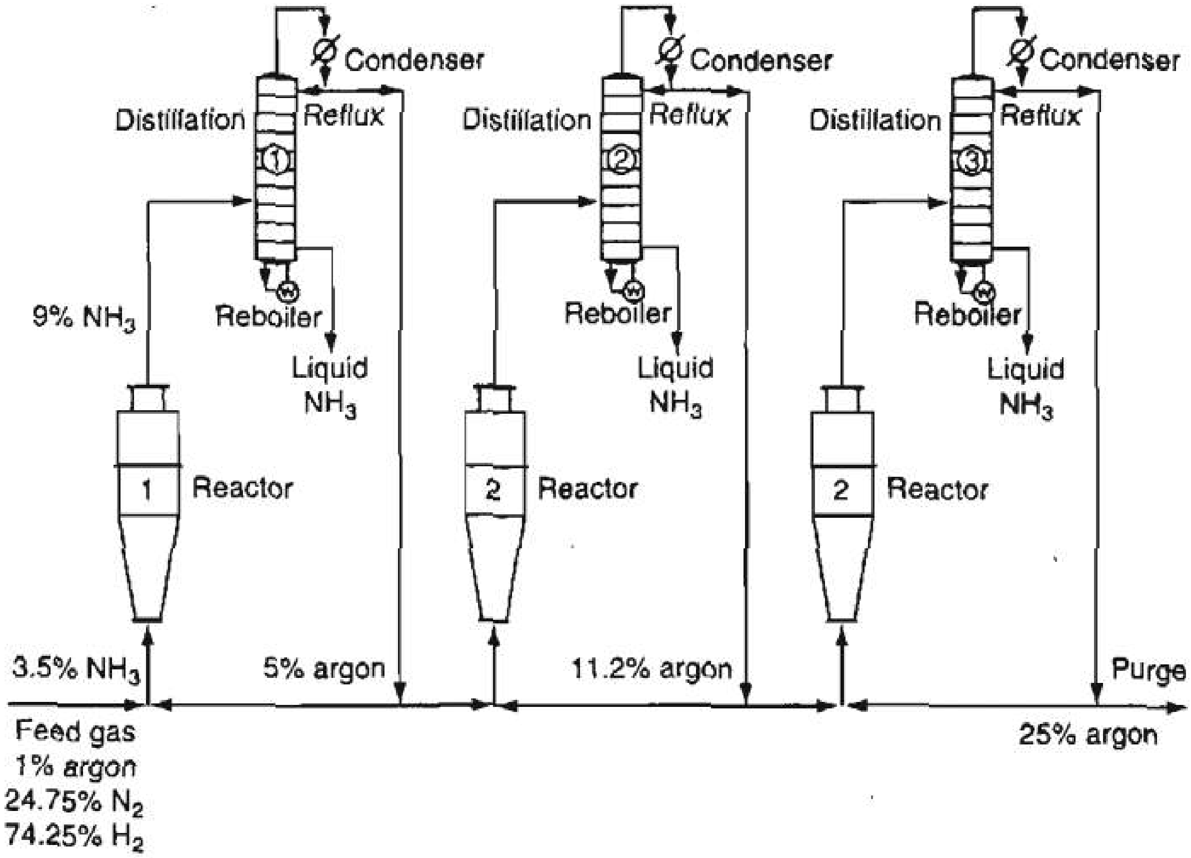
Some of the important applications of bypass stream are as follow:

1. Pumping of liquid from a storage tank by a more efficient pump of high horsepower to a small process unit at desired lower flow rate.
2. Dissolution of caustic soda (NaOH) in water by two steps process due to the very high heat of dissolution.
3. Separation of mixtures by a more efficient distillation column, so that a bypass stream is used to control the composition of the product at the desired value.

b. **Purge stream:** It is a fraction of the recycle stream (with the same composition) that is removed out the process to prevent accumulation of inert materials (that are not involve in the reaction) in the recycle stream so that the quantity of inert input within the fresh feed is equal to that output with the purge stream as shown in the following block diagram.

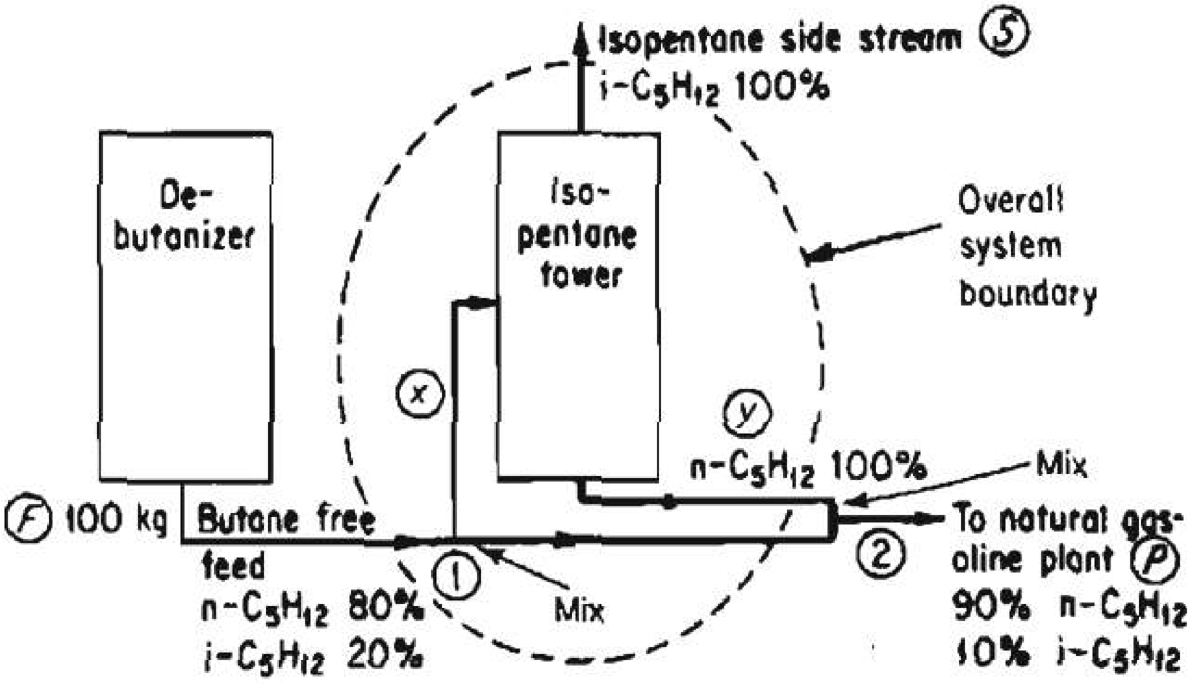


* The important example of application of purge stream is in the production of ammonia from gaseous mixture of N_2 and H_2 containing some impurities of argon as shown in the following block diagram.



Note how in the steady state the argon concentration is different in each successive recycle stream so that 1% argon occurs in the feed stream while, 25% argon occurs in the third recycle and purge stream. For effective operation, the Argon concentration cannot be allowed to increase further. Remember that the process operates continuously in the steady state so that the Argon concentration is constant in each individual recycle stream.

Example 12.5: Isopentane is removed from butane-free gasoline to use it in plant of natural gasoline as shown in figure below. What fraction of the butane-free gasoline is passed through the isopentane tower? The process is in the steady state and no reaction occurs.



Solution:

Basis: 100 kg feed

Overall material balance:

F = S + P
100 = S + P ………………………………….(1)

Overall material balance on n-C_5H_{12} (Tie component):

100 (0.8) = S (0) + P (0.9)
P = 88.9 kg
From Eq.(1):
S = 100 – 88.9 = 11.1 kg

Overall material balance around isopentane tower:

Let: x = kg of butane free gasoline going to the isopentane tower.
y = kg of n-C_5H_{12} stream leaving the isopentane tower.
x = S + y
x = 11.1 + y ………………………(2)

Component material balance for n-C_5H_{12} around isopentane tower:

x (0.8) = y …………………………(3)

From Eq.(2) and Eq.(3):

x = 55.5 kg

The desired fraction = (55.5 / 100) =0.555

Another solution of this problem:

Overall material balance around mixing point:

y + bypass stream = P

y + (100 – x) = 88.9 …………………… (4)

i-C_5H_{12} material balance around mixing point:

(100 – x) (0.2) + 0 = 88.9 (0.1)

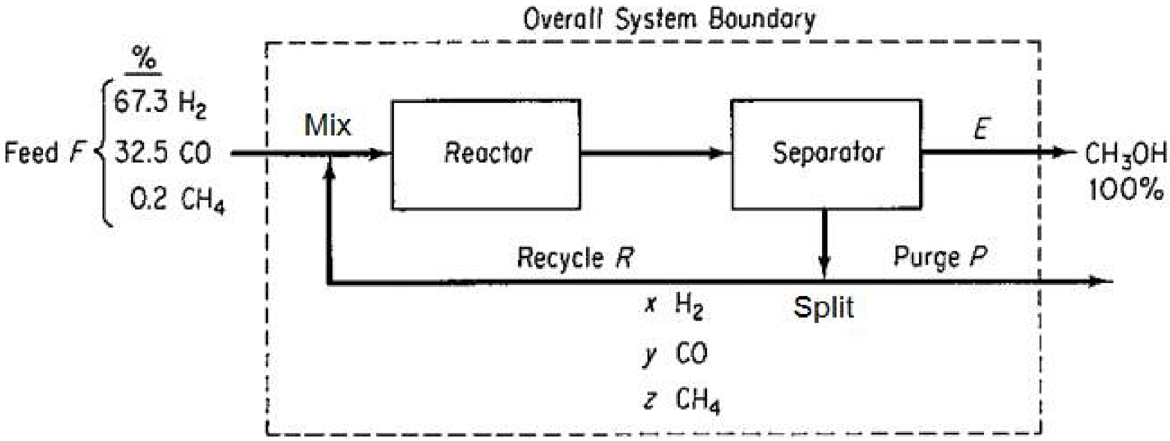
x = 55.5 kg

y = 44.5 kg

Example 12.6: Two gases CO and H_2 can be combined under suitable conditions to yield methanol according to the following equation

$CO + 2H_2 \rightarrow CH_3OH$

Figure below illustrates a steady-state process for the production of methanol. All of the compositions are in mole fractions and the stream flows are in moles.



Note in Figure above that some CH_4 enters the process, but does not participate in the reaction. A purge stream is used to maintain the CH_4 concentration in the exit from the separator at no more than 3.2 mol%, and prevent hydrogen buildup as well. The once-through conversion of the CO in the reactor is 18%. Compute the moles of recycle, CH_3OH, and purge per mole of feed, and also compute the purge gas composition.

Solution:

Basis: 100 kgmol feed

The purge and recycle streams have the same composition. Assume that the purge stream contains the maximum allowed CH_4.

$z = 3.2\% = 0.032$ …………………………(1)

Total mole fraction = 1

$x + y + z = 1$ ………………………………..(2)

<u>The overall element material balances are in (moles):</u>

Input = Output

H_2: $67.3 + 2\,(0.2) = E\,(2) + P\,(x + 2z)$ …………………(3)
C: $32.5 + 0.2 = E\,(1) + P\,(y + z)$ ………………………..(4)
O: $32.5 = E\,(1) + P\,(1)$ …………………………………(5)

<u>CO material balance:</u>

The single –pass conversion for CO:

$$f_{sp}\ (\mathrm{CO}) = \frac{moles\ of\ reactant\ fed\ into\ the\ reactor - moles\ of\ reactant\ exiting\ the\ reactor}{moles\ \ of\ reactant\ fed\ into\ the\ reactor}$$

$$0.18 = \frac{(32.5+\mathrm{R}\ \mathrm{y})-[\,y\ (\mathrm{R}+\mathrm{P})]}{(32.5+\mathrm{R}\ \mathrm{y})} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.\ldots\ (6)$$

We have six equations and six unknown variables, by successive substitution or by using computer program. The resulting values obtained are in moles:

E CH_3OH = 31.25 mole
P Purge = 6.25 mole
R Recycle = 705 mole
x H_2 = 0.768
y CO = 0.2
z CH_4 = 0.032

<u>H.W.</u> Problem 1, Problem 2 page 364-365
Problem 1, Problem 2 page 371-372
12.2, 12.3, 12.4, 12.7,